Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:41 AM EDT

PDB ID	:	1YCH / pdb_00001ych
Title	:	X-ray Crystal Structures of Moorella thermoacetica FprA. Novel Diiron Site Structure and Mechanistic Insights into a Scavenging Nitric Oxide Reductase
Authors	:	Silaghi-Dumitrescu, R.; Kurtz, D.M.; Lanzilotta, W.N.
Deposited on	:	2004-12-22
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

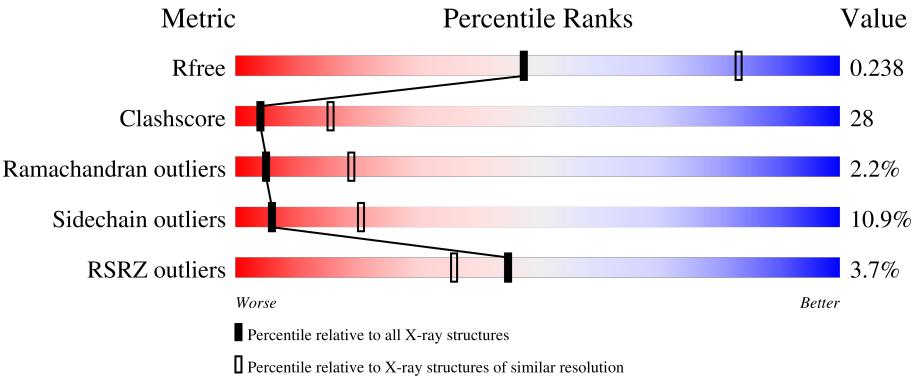
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	4% 52% 35% 12%
1	B	398	5% 52% 37% 10%
1	C	398	3% 59% 32% 8%
1	D	398	4% 54% 34% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12886 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

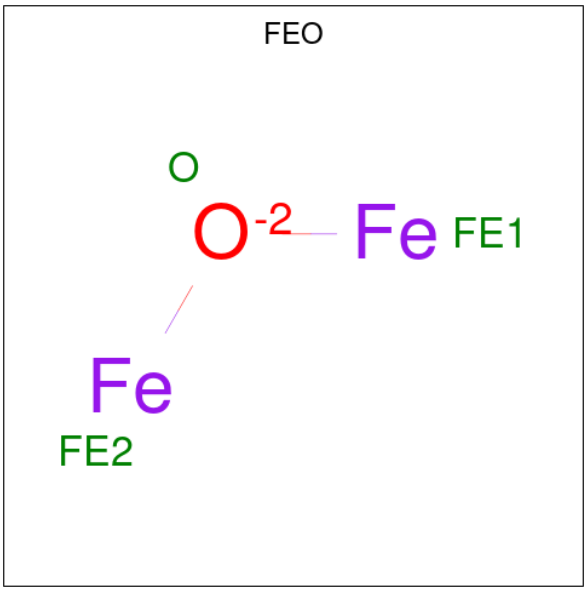
- Molecule 1 is a protein called Nitric oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	B	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	C	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	D	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

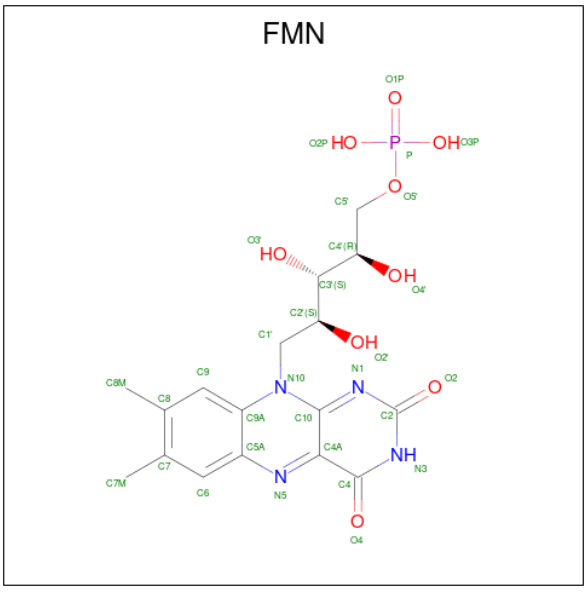
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe O 3 2 1	0	0
3	B	1	Total Fe O 3 2 1	0	0
3	C	1	Total Fe O 3 2 1	0	0
3	D	1	Total Fe O 3 2 1	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is water.

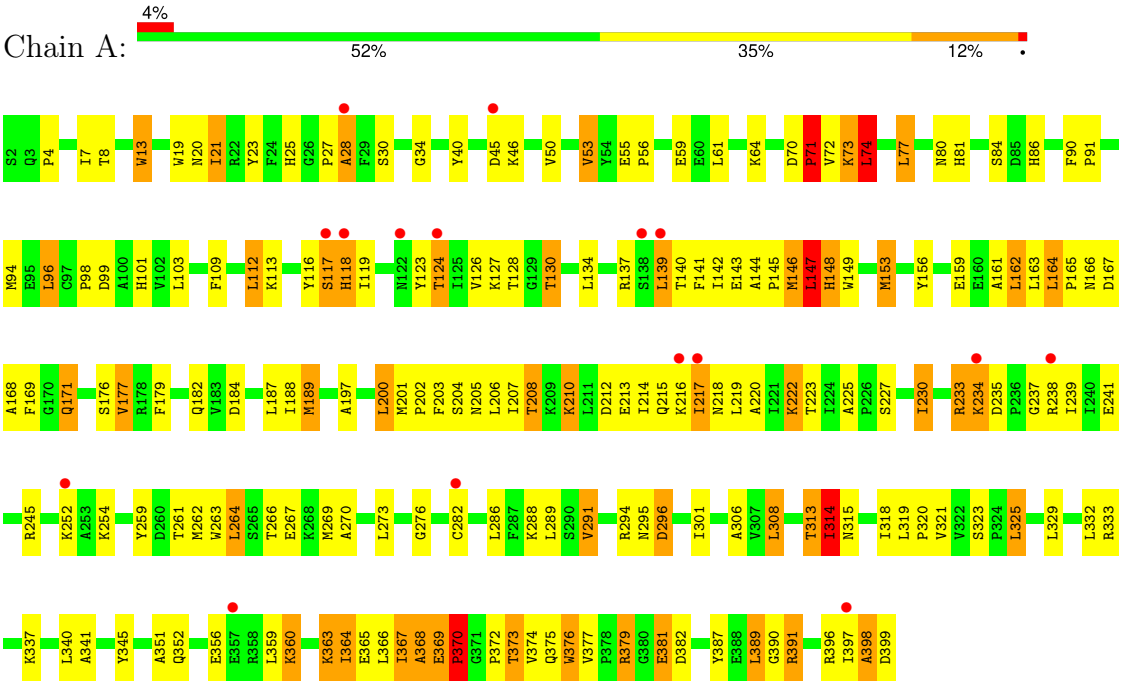
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	B	57	Total	O	0	0
			57	57		
5	C	87	Total	O	0	0
			87	87		
5	D	70	Total	O	0	0
			70	70		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

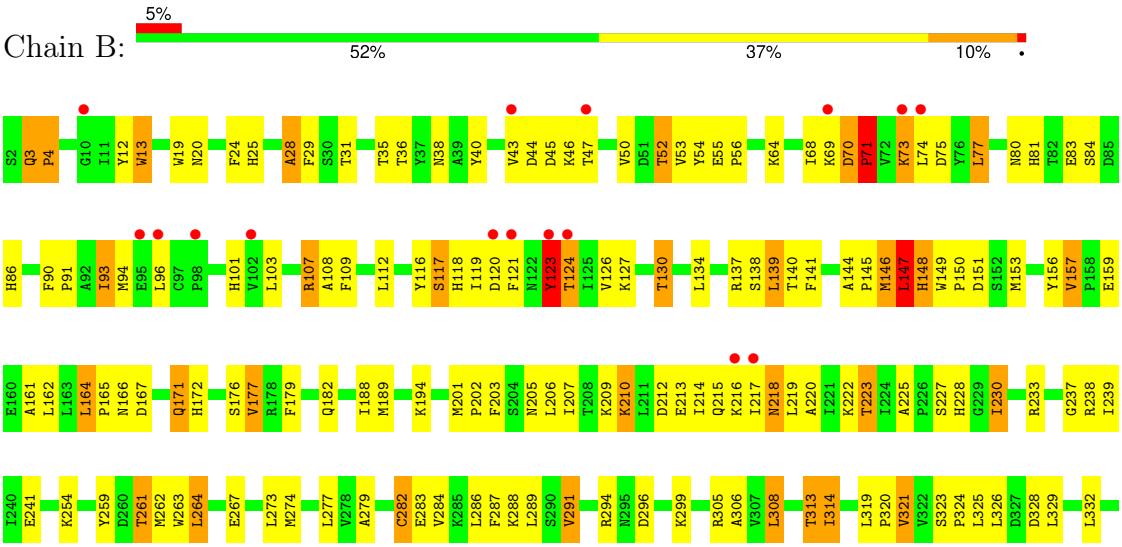
• Molecule 1: Nitric oxide reductase

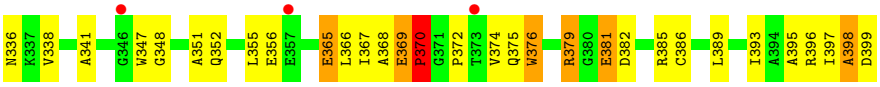
Chain A:



• Molecule 1: Nitric oxide reductase

Chain B:

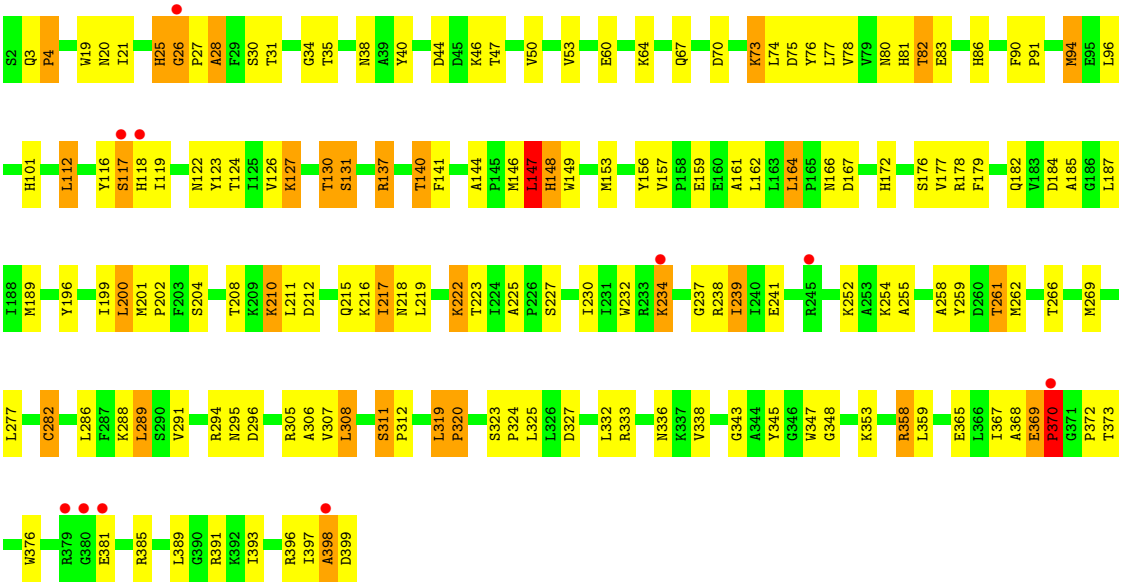




• Molecule 1: Nitric oxide reductase

Chain C:

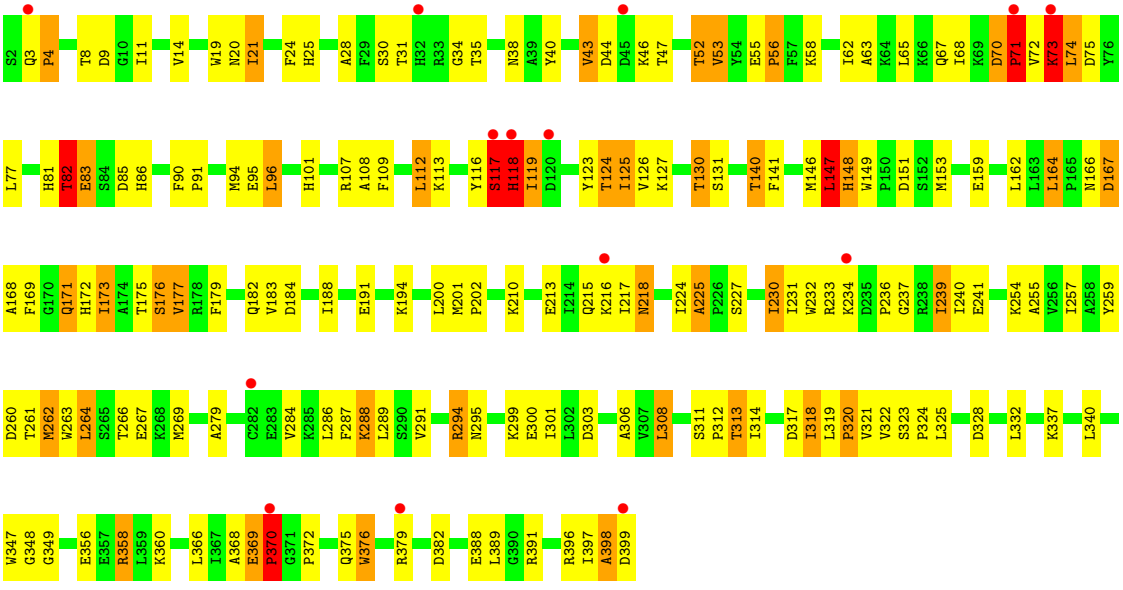




• Molecule 1: Nitric oxide reductase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	160.33Å 160.33Å 279.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.91 – 2.80 43.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.91-2.80) 99.2 (43.91-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.245 0.218 , 0.238	Depositor DCC
R_{free} test set	4464 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12886	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FEO, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.99	5/3189 (0.2%)	1.63	37/4335 (0.9%)
1	B	1.03	3/3189 (0.1%)	1.57	34/4335 (0.8%)
1	C	1.01	3/3189 (0.1%)	1.38	39/4335 (0.9%)
1	D	1.04	2/3189 (0.1%)	1.41	40/4335 (0.9%)
All	All	1.02	13/12756 (0.1%)	1.50	150/17340 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLU	C-O	8.34	1.36	1.23
1	D	73	LYS	C-O	-7.74	1.10	1.23
1	C	369	GLU	CA-C	7.31	1.61	1.53
1	D	118	HIS	CA-C	6.74	1.61	1.52
1	A	153	MET	SD-CE	6.66	1.96	1.79
1	A	262	MET	SD-CE	6.57	1.96	1.79
1	C	94	MET	SD-CE	-6.53	1.63	1.79
1	A	21	ILE	CA-CB	5.79	1.60	1.54
1	C	262	MET	SD-CE	5.78	1.94	1.79
1	B	146	MET	SD-CE	5.74	1.94	1.79
1	A	146	MET	SD-CE	5.57	1.93	1.79
1	B	120	ASP	CB-CG	5.16	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	MET	SD-CE	5.11	1.92	1.79

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ASP	CA-C-N	47.62	179.37	119.84
1	A	70	ASP	C-N-CA	47.62	179.37	119.84
1	B	70	ASP	CA-C-N	44.83	175.88	119.84
1	B	70	ASP	C-N-CA	44.83	175.88	119.84
1	D	70	ASP	CA-C-N	21.16	177.78	127.00
1	D	70	ASP	C-N-CA	21.16	177.78	127.00
1	C	369	GLU	CA-C-N	20.70	145.72	119.84
1	C	369	GLU	C-N-CA	20.70	145.72	119.84
1	D	70	ASP	C-N-CD	-19.70	77.26	120.60
1	C	369	GLU	C-N-CD	-13.47	69.78	125.00
1	B	70	ASP	C-N-CD	-12.12	75.31	125.00
1	C	370	PRO	N-CA-C	-11.78	88.21	112.47
1	C	70	ASP	C-N-CD	-11.45	95.40	120.60
1	C	70	ASP	CA-C-N	10.69	152.64	127.00
1	C	70	ASP	C-N-CA	10.69	152.64	127.00
1	A	70	ASP	C-N-CD	-10.68	81.19	125.00
1	D	147	LEU	N-CA-C	-10.18	96.53	110.68
1	A	147	LEU	N-CA-C	-9.91	96.90	110.68
1	A	71	PRO	CA-N-CD	-9.77	98.33	112.00
1	C	147	LEU	N-CA-C	-9.69	97.21	110.68
1	A	369	GLU	CA-C-N	8.99	131.08	119.84
1	A	369	GLU	C-N-CA	8.99	131.08	119.84
1	A	369	GLU	N-CA-C	-8.98	99.27	109.60
1	B	147	LEU	N-CA-C	-8.86	98.36	110.68
1	D	369	GLU	CA-C-N	8.81	130.86	119.84
1	D	369	GLU	C-N-CA	8.81	130.86	119.84
1	D	369	GLU	N-CA-C	-8.79	98.48	109.64
1	C	369	GLU	N-CA-C	-8.79	98.67	109.83
1	A	369	GLU	C-N-CD	-8.76	89.09	125.00
1	B	84	SER	N-CA-C	8.71	121.92	111.82
1	A	164	LEU	CA-C-N	8.45	129.50	120.12
1	A	164	LEU	C-N-CA	8.45	129.50	120.12
1	D	289	LEU	N-CA-C	8.38	121.47	111.33
1	D	369	GLU	C-N-CD	-8.37	90.68	125.00
1	D	74	LEU	N-CA-C	8.28	122.44	110.10
1	A	289	LEU	N-CA-C	8.19	122.23	111.75
1	B	289	LEU	N-CA-C	8.07	121.09	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	289	LEU	N-CA-C	7.64	121.53	111.75
1	B	71	PRO	CA-N-CD	-7.34	101.72	112.00
1	B	20	ASN	N-CA-C	7.06	121.92	113.16
1	D	370	PRO	N-CA-C	-6.85	98.36	112.47
1	C	176	SER	N-CA-C	-6.77	105.02	113.28
1	C	20	ASN	N-CA-C	6.76	121.53	113.28
1	D	20	ASN	N-CA-C	6.69	121.44	113.28
1	C	147	LEU	CA-C-N	6.63	134.21	121.54
1	C	147	LEU	C-N-CA	6.63	134.21	121.54
1	D	176	SER	N-CA-C	-6.57	105.26	113.28
1	C	164	LEU	CA-C-N	6.55	127.72	120.45
1	C	164	LEU	C-N-CA	6.55	127.72	120.45
1	B	179	PHE	N-CA-C	6.52	120.32	109.95
1	C	179	PHE	N-CA-C	6.46	120.22	109.95
1	D	147	LEU	CA-C-N	6.45	133.86	121.54
1	D	147	LEU	C-N-CA	6.45	133.86	121.54
1	D	123	TYR	N-CA-C	6.42	117.05	108.38
1	A	45	ASP	N-CA-C	-6.40	103.59	111.33
1	C	370	PRO	CA-N-CD	-6.32	103.15	112.00
1	C	123	TYR	N-CA-C	6.30	116.89	108.38
1	A	179	PHE	N-CA-C	6.28	119.93	109.95
1	C	288	LYS	N-CA-C	-6.26	98.33	108.41
1	D	288	LYS	N-CA-C	-6.25	98.35	108.41
1	C	311	SER	CA-C-N	6.24	127.65	120.98
1	C	311	SER	C-N-CA	6.24	127.65	120.98
1	B	369	GLU	C-N-CD	-6.18	99.67	125.00
1	B	83	GLU	N-CA-C	-6.15	102.40	110.33
1	B	288	LYS	N-CA-C	-6.14	98.52	108.41
1	A	20	ASN	N-CA-C	6.14	120.93	113.38
1	B	164	LEU	CA-C-N	6.12	126.92	120.12
1	B	164	LEU	C-N-CA	6.12	126.92	120.12
1	B	3	GLN	CA-C-N	6.10	126.07	120.03
1	B	3	GLN	C-N-CA	6.10	126.07	120.03
1	A	19	TRP	N-CA-C	6.08	117.98	111.36
1	A	28	ALA	N-CA-C	6.08	121.33	111.37
1	D	83	GLU	CA-C-N	-6.06	111.41	122.38
1	D	83	GLU	C-N-CA	-6.06	111.41	122.38
1	D	167	ASP	N-CA-C	6.04	117.86	111.28
1	D	225	ALA	CA-C-N	5.96	125.93	120.21
1	D	225	ALA	C-N-CA	5.96	125.93	120.21
1	B	19	TRP	N-CA-C	5.95	117.77	111.28
1	A	296	ASP	N-CA-C	-5.94	104.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	19	TRP	N-CA-C	5.92	117.81	111.36
1	D	19	TRP	N-CA-C	5.91	117.72	111.28
1	D	68	ILE	N-CA-C	-5.91	105.32	111.58
1	B	264	LEU	N-CA-C	5.90	122.48	113.51
1	B	13	TRP	N-CA-C	-5.89	99.67	109.46
1	C	157	VAL	CA-C-N	5.89	127.20	119.84
1	C	157	VAL	C-N-CA	5.89	127.20	119.84
1	B	176	SER	N-CA-C	-5.88	105.87	113.16
1	B	45	ASP	N-CA-C	-5.87	104.23	111.33
1	B	157	VAL	CA-C-N	5.74	127.02	119.84
1	B	157	VAL	C-N-CA	5.74	127.02	119.84
1	C	28	ALA	N-CA-C	5.74	120.78	111.37
1	A	147	LEU	CA-C-N	5.69	132.41	121.54
1	A	147	LEU	C-N-CA	5.69	132.41	121.54
1	D	73	LYS	O-C-N	-5.68	113.08	121.89
1	A	370	PRO	N-CA-C	-5.67	100.78	112.47
1	D	82	THR	N-CA-C	5.66	119.88	112.92
1	D	124	THR	CB-CA-C	-5.63	102.02	110.24
1	B	147	LEU	CA-C-N	5.62	132.27	121.54
1	B	147	LEU	C-N-CA	5.62	132.27	121.54
1	C	178	ARG	N-CA-C	5.61	121.15	113.97
1	D	52	THR	CA-C-O	5.60	121.86	118.33
1	C	82	THR	N-CA-C	5.58	119.40	112.59
1	C	4	PRO	N-CA-C	-5.56	103.44	111.22
1	D	370	PRO	CA-N-CD	-5.56	104.22	112.00
1	D	71	PRO	CA-N-CD	-5.53	103.75	111.50
1	B	28	ALA	N-CA-C	5.50	120.40	111.37
1	D	179	PHE	N-CA-C	5.50	118.53	109.72
1	A	13	TRP	N-CA-C	-5.50	100.33	109.46
1	A	264	LEU	N-CA-C	5.50	121.86	113.51
1	D	119	ILE	CB-CA-C	-5.47	103.03	110.42
1	A	167	ASP	N-CA-C	5.47	117.33	111.36
1	B	123	TYR	N-CA-C	5.45	115.74	108.38
1	D	262	MET	N-CA-C	-5.44	106.69	113.55
1	A	176	SER	N-CA-C	-5.41	106.68	113.28
1	A	370	PRO	CA-N-CD	-5.41	104.42	112.00
1	D	52	THR	CB-CA-C	-5.40	108.60	116.53
1	A	46	LYS	N-CA-C	-5.39	100.61	109.40
1	C	199	ILE	N-CA-C	5.39	116.20	111.56
1	A	71	PRO	N-CA-C	-5.39	101.36	112.47
1	A	200	LEU	N-CA-C	5.39	119.86	113.28
1	D	164	LEU	CA-C-N	5.39	126.10	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	164	LEU	C-N-CA	5.39	126.10	120.12
1	B	71	PRO	N-CA-C	-5.39	101.37	112.47
1	A	123	TYR	N-CA-C	5.38	115.65	108.38
1	A	262	MET	N-CA-C	-5.34	106.83	113.55
1	D	4	PRO	N-CA-C	-5.33	103.42	111.41
1	B	264	LEU	N-CA-CB	-5.31	108.79	114.10
1	A	197	ALA	N-CA-C	5.30	117.06	111.28
1	A	74	LEU	N-CA-C	5.27	122.02	110.80
1	A	288	LYS	N-CA-C	-5.26	100.52	108.67
1	C	369	GLU	CB-CA-C	5.25	117.66	109.42
1	C	320	PRO	N-CA-C	5.23	120.64	113.84
1	B	4	PRO	N-CA-C	-5.19	103.62	111.41
1	C	368	ALA	CA-C-N	-5.18	113.14	120.49
1	C	368	ALA	C-N-CA	-5.18	113.14	120.49
1	D	231	ILE	CB-CA-C	-5.18	104.69	110.96
1	A	314	ILE	CB-CA-C	-5.16	102.94	110.62
1	C	200	LEU	N-CA-C	5.15	119.57	113.28
1	A	7	ILE	N-CA-C	-5.15	105.09	112.35
1	C	26	GLY	CA-C-N	5.14	126.26	119.84
1	C	26	GLY	C-N-CA	5.14	126.26	119.84
1	B	287	PHE	N-CA-C	5.12	116.76	108.41
1	A	4	PRO	N-CA-C	-5.09	104.10	111.22
1	D	264	LEU	N-CA-C	5.06	121.20	113.51
1	B	52	THR	CA-C-O	5.06	121.52	118.33
1	B	282	CYS	N-CA-CB	-5.04	102.58	110.69
1	B	365	GLU	N-CA-C	5.02	116.38	109.15
1	C	296	ASP	N-CA-C	-5.02	106.00	111.82
1	C	25	HIS	CB-CA-C	-5.01	104.78	111.89
1	D	200	LEU	N-CA-C	5.01	119.39	113.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	TYR	Sidechain
1	B	259	TYR	Sidechain
1	C	196	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3115	0	3131	196	0
1	B	3115	0	3131	205	0
1	C	3115	0	3131	147	0
1	D	3115	0	3131	172	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	31	0	19	0	0
4	B	31	0	19	2	0
4	C	31	0	19	2	0
4	D	31	0	19	0	0
5	A	68	0	0	15	0
5	B	57	0	0	28	0
5	C	87	0	0	11	0
5	D	70	0	0	10	0
All	All	12886	0	12600	693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:HB3	1:A:370:PRO:HD2	1.19	1.17
1:B:381:GLU:CD	1:B:381:GLU:H	1.54	1.16
1:D:369:GLU:HB3	1:D:370:PRO:HD2	1.25	1.16
1:A:261:THR:HG22	1:A:266:THR:HB	1.19	1.15
1:C:25:HIS:HB3	1:D:262:MET:HE2	1.31	1.10
1:B:369:GLU:HG3	1:B:370:PRO:HD2	1.33	1.07
1:B:314:ILE:HD11	1:B:319:LEU:HA	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLU:H	1:A:381:GLU:CD	1.61	1.05
1:D:261:THR:HG22	1:D:266:THR:HB	1.40	1.02
1:D:201:MET:HE2	1:D:332:LEU:HB3	1.43	1.01
1:A:234:LYS:HE3	1:A:234:LYS:HA	1.39	1.00
1:D:109:PHE:CE2	1:D:113:LYS:HE2	1.98	0.98
1:B:171:GLN:HE22	1:B:230:ILE:H	1.14	0.95
1:A:333:ARG:HH11	1:A:363:LYS:HZ3	1.02	0.94
1:A:171:GLN:HE22	1:A:230:ILE:H	1.16	0.94
1:B:381:GLU:CD	1:B:381:GLU:N	2.25	0.94
1:D:171:GLN:HE22	1:D:230:ILE:H	1.06	0.94
1:B:202:PRO:HG3	1:B:332:LEU:HA	1.48	0.93
1:D:369:GLU:CB	1:D:370:PRO:HD2	1.95	0.93
1:B:314:ILE:HD11	1:B:319:LEU:CA	1.99	0.92
1:B:127:LYS:H	1:B:130:THR:CG2	1.83	0.92
1:A:314:ILE:HD11	1:A:319:LEU:HA	1.48	0.92
1:C:234:LYS:HE3	1:C:234:LYS:HA	1.52	0.92
1:D:71:PRO:HD2	1:D:71:PRO:O	1.68	0.91
1:B:69:LYS:HG3	5:B:756:HOH:O	1.70	0.91
1:A:117:SER:O	1:A:119:ILE:N	2.03	0.90
1:D:318:ILE:HD11	1:D:322:VAL:HB	1.53	0.90
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.35	0.90
1:A:320:PRO:HG2	1:B:294:ARG:HH12	1.37	0.89
1:A:25:HIS:HB3	1:B:262:MET:HE3	1.53	0.89
1:A:77:LEU:HD12	1:A:94:MET:HE1	1.54	0.87
1:C:261:THR:HG22	4:C:721:FMN:O1P	1.75	0.87
1:C:127:LYS:H	1:C:130:THR:CG2	1.88	0.86
1:D:306:ALA:HB2	1:D:397:ILE:HD11	1.54	0.86
1:A:127:LYS:O	1:A:130:THR:HG23	1.74	0.86
1:D:318:ILE:CD1	1:D:322:VAL:HB	2.05	0.86
1:A:381:GLU:CD	1:A:381:GLU:N	2.33	0.85
1:D:43:VAL:HA	1:D:47:THR:HG22	1.58	0.85
1:B:305:ARG:HB3	1:B:397:ILE:HD12	1.59	0.85
1:A:127:LYS:H	1:A:130:THR:CG2	1.90	0.85
1:B:372:PRO:HG3	1:B:389:LEU:CD1	2.08	0.83
1:B:379:ARG:HB2	1:B:381:GLU:OE2	1.78	0.83
1:B:369:GLU:CG	1:B:370:PRO:HD2	2.06	0.83
1:A:369:GLU:CB	1:A:370:PRO:HD2	1.88	0.83
1:C:127:LYS:H	1:C:130:THR:HG21	1.44	0.83
1:A:261:THR:CG2	1:A:266:THR:HB	2.07	0.82
1:B:313:THR:HG22	1:B:351:ALA:HB3	1.62	0.82
1:A:379:ARG:HG3	1:A:381:GLU:OE2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LYS:O	1:C:305:ARG:HG3	1.80	0.81
1:A:294:ARG:NH1	1:B:320:PRO:HB2	1.95	0.81
1:A:189:MET:HE2	5:A:741:HOH:O	1.80	0.81
1:B:107:ARG:HB3	1:B:107:ARG:NH1	1.95	0.81
1:D:261:THR:CG2	1:D:266:THR:HB	2.10	0.81
1:B:117:SER:O	1:B:119:ILE:N	2.14	0.80
1:D:117:SER:O	1:D:119:ILE:N	2.14	0.80
1:B:347:TRP:CD1	1:B:348:GLY:H	1.99	0.80
1:A:320:PRO:HG2	1:B:294:ARG:NH1	1.96	0.80
1:C:261:THR:HG23	1:C:266:THR:HB	1.63	0.80
1:A:72:VAL:CG1	1:A:74:LEU:HD13	2.13	0.79
1:A:127:LYS:H	1:A:130:THR:HG21	1.48	0.79
1:B:147:LEU:HD11	5:B:753:HOH:O	1.82	0.79
1:B:314:ILE:CD1	1:B:319:LEU:HA	2.12	0.79
1:A:269:MET:HE2	1:A:374:VAL:HB	1.65	0.78
1:A:314:ILE:HD11	1:A:319:LEU:CA	2.14	0.78
1:C:117:SER:O	1:C:119:ILE:N	2.17	0.78
1:B:101:HIS:NE2	1:B:124:THR:HG22	1.97	0.78
1:A:333:ARG:HD2	1:A:363:LYS:HE2	1.63	0.78
1:B:141:PHE:HB3	1:B:153:MET:CE	2.13	0.78
1:A:360:LYS:HE3	1:A:369:GLU:OE2	1.85	0.77
1:D:306:ALA:CB	1:D:397:ILE:HD11	2.15	0.77
1:C:90:PHE:CE1	1:C:94:MET:HE3	2.20	0.76
1:A:333:ARG:HD2	1:A:363:LYS:CE	2.15	0.76
1:A:72:VAL:HB	1:A:96:LEU:HD11	1.67	0.76
1:B:338:VAL:HG11	1:B:367:ILE:HD13	1.68	0.76
1:C:259:TYR:HE2	1:C:286:LEU:HD21	1.51	0.76
1:B:127:LYS:H	1:B:130:THR:HG21	1.49	0.75
1:D:127:LYS:O	1:D:130:THR:HG23	1.86	0.75
1:D:372:PRO:HG3	1:D:389:LEU:CD1	2.16	0.75
1:B:141:PHE:HB3	1:B:153:MET:HE1	1.69	0.75
1:D:202:PRO:HG3	1:D:332:LEU:HA	1.67	0.75
1:D:171:GLN:HE22	1:D:230:ILE:N	1.83	0.74
1:C:127:LYS:O	1:C:130:THR:HG22	1.86	0.74
1:D:82:THR:HG22	1:D:112:LEU:HD13	1.70	0.73
1:C:30:SER:H	1:C:295:ASN:ND2	1.85	0.73
1:B:356:GLU:HG2	1:B:366:LEU:CD1	2.19	0.73
1:D:8:THR:CG2	1:D:11:ILE:HD13	2.18	0.73
1:D:188:ILE:HD11	1:D:230:ILE:HB	1.71	0.73
1:D:259:TYR:HE2	1:D:286:LEU:HD21	1.52	0.73
1:A:340:LEU:HD11	1:A:372:PRO:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HA	1:A:159:GLU:HG2	1.70	0.73
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.00	0.73
1:B:372:PRO:HG3	1:B:389:LEU:HD13	1.69	0.72
1:A:372:PRO:HG3	1:A:389:LEU:HD13	1.71	0.72
1:D:127:LYS:H	1:D:130:THR:CG2	2.02	0.72
1:C:381:GLU:OE1	1:C:381:GLU:N	2.14	0.72
1:A:270:ALA:HB1	5:A:746:HOH:O	1.89	0.72
1:B:126:VAL:HG13	1:B:130:THR:HG23	1.72	0.72
1:A:202:PRO:HG3	1:A:332:LEU:HA	1.71	0.71
1:D:3:GLN:OE1	1:D:67:GLN:NE2	2.24	0.71
1:C:369:GLU:HG2	1:C:370:PRO:HD3	1.70	0.71
1:D:318:ILE:HD11	1:D:322:VAL:CB	2.20	0.71
1:D:101:HIS:HE1	1:D:124:THR:OG1	1.74	0.71
1:B:305:ARG:HB2	1:B:397:ILE:HG23	1.72	0.70
1:B:70:ASP:OD1	1:B:71:PRO:HD3	1.91	0.70
1:B:159:GLU:OE1	5:B:766:HOH:O	2.08	0.70
1:C:312:PRO:HD2	1:C:319:LEU:HD22	1.74	0.70
1:B:96:LEU:HD13	1:B:96:LEU:O	1.91	0.70
1:A:25:HIS:CB	1:B:262:MET:HE3	2.22	0.70
1:C:101:HIS:HE1	1:C:124:THR:OG1	1.74	0.69
1:A:269:MET:CE	1:A:374:VAL:HB	2.22	0.69
1:B:43:VAL:HA	1:B:47:THR:HG22	1.73	0.69
1:C:261:THR:CG2	1:C:266:THR:HB	2.22	0.69
1:C:372:PRO:HG3	1:C:389:LEU:HD12	1.75	0.69
1:A:77:LEU:HD12	1:A:94:MET:CE	2.22	0.69
1:B:127:LYS:O	1:B:130:THR:HG23	1.93	0.68
1:B:202:PRO:HG3	1:B:332:LEU:CA	2.21	0.68
1:D:308:LEU:HD13	1:D:340:LEU:HB3	1.76	0.68
1:B:207:ILE:HG12	5:B:753:HOH:O	1.94	0.68
1:C:269:MET:HE1	1:C:343:GLY:C	2.18	0.68
1:D:201:MET:CE	1:D:332:LEU:HB3	2.23	0.68
1:B:90:PHE:CE1	1:B:94:MET:CE	2.76	0.68
1:B:107:ARG:HB3	1:B:107:ARG:HH11	1.57	0.68
1:C:365:GLU:OE1	1:C:396:ARG:NH2	2.26	0.68
1:B:46:LYS:HA	1:B:75:ASP:OD2	1.93	0.68
1:C:146:MET:C	1:C:148:HIS:H	2.01	0.68
1:A:146:MET:C	1:A:148:HIS:H	2.02	0.68
1:C:3:GLN:OE1	1:C:67:GLN:NE2	2.27	0.68
1:A:313:THR:HG22	1:A:351:ALA:HB3	1.76	0.68
1:D:65:LEU:HA	5:D:796:HOH:O	1.93	0.68
1:C:126:VAL:HG13	1:C:130:THR:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PRO:HG3	1:C:332:LEU:HA	1.75	0.67
1:A:234:LYS:HA	1:A:234:LYS:CE	2.22	0.67
1:B:139:LEU:HG	5:B:752:HOH:O	1.95	0.67
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.09	0.67
1:D:146:MET:C	1:D:148:HIS:H	2.01	0.67
1:A:159:GLU:CD	1:A:159:GLU:H	2.03	0.67
1:B:141:PHE:CD2	1:B:153:MET:HE1	2.30	0.67
1:A:379:ARG:HH11	1:A:382:ASP:CG	2.03	0.66
1:D:82:THR:CG2	1:D:112:LEU:HD13	2.25	0.66
1:C:90:PHE:HB3	1:C:91:PRO:HD3	1.77	0.66
1:C:320:PRO:HB2	1:D:294:ARG:NH1	2.11	0.66
1:D:262:MET:HE1	1:D:314:ILE:HD12	1.77	0.66
1:A:263:TRP:O	1:A:264:LEU:HB2	1.94	0.66
1:B:138:SER:N	1:B:159:GLU:OE1	2.27	0.66
1:B:277:LEU:O	1:B:282:CYS:HB3	1.96	0.66
1:A:308:LEU:HD13	1:A:340:LEU:HB3	1.77	0.65
1:D:58:LYS:HA	5:D:740:HOH:O	1.96	0.65
1:B:296:ASP:HA	5:B:750:HOH:O	1.94	0.65
1:D:8:THR:HG23	1:D:11:ILE:HD13	1.78	0.65
1:A:90:PHE:HB3	1:A:91:PRO:HD3	1.78	0.65
1:B:262:MET:HE1	4:B:711:FMN:C8M	2.27	0.65
1:B:25:HIS:HB2	1:B:28:ALA:HB3	1.79	0.64
1:C:204:SER:OG	5:C:749:HOH:O	2.15	0.64
1:A:379:ARG:CG	1:A:381:GLU:OE2	2.45	0.64
1:B:146:MET:C	1:B:148:HIS:H	2.05	0.64
1:B:157:VAL:C	5:B:766:HOH:O	2.39	0.64
1:D:261:THR:HG22	1:D:266:THR:CB	2.23	0.64
1:A:398:ALA:O	1:A:399:ASP:CB	2.45	0.64
1:B:148:HIS:HD2	1:B:167:ASP:OD2	1.80	0.64
1:A:118:HIS:ND1	1:D:388:GLU:OE2	2.26	0.64
1:B:126:VAL:HG11	1:B:141:PHE:CG	2.32	0.64
1:C:82:THR:HG22	1:C:112:LEU:HD13	1.80	0.64
1:B:313:THR:HG22	1:B:351:ALA:CB	2.27	0.63
1:B:305:ARG:CB	1:B:397:ILE:HG23	2.27	0.63
1:D:372:PRO:HG3	1:D:389:LEU:HD12	1.78	0.63
1:B:44:ASP:H	1:B:47:THR:HG22	1.63	0.63
1:C:294:ARG:HH12	1:D:320:PRO:HG2	1.62	0.63
1:D:173:ILE:CD1	1:D:175:THR:HG23	2.27	0.63
1:B:126:VAL:HG13	1:B:130:THR:CG2	2.29	0.63
1:D:44:ASP:H	1:D:47:THR:HG22	1.64	0.63
1:D:318:ILE:HD11	1:D:322:VAL:CG1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TYR:CE1	1:B:219:LEU:HD22	2.32	0.63
1:D:25:HIS:HB2	1:D:28:ALA:HB3	1.81	0.63
1:D:71:PRO:O	1:D:71:PRO:CD	2.44	0.62
1:B:203:PHE:O	5:B:753:HOH:O	2.16	0.62
1:A:40:TYR:CZ	1:A:225:ALA:HB1	2.34	0.62
1:A:139:LEU:HD13	1:A:141:PHE:CZ	2.34	0.62
1:B:90:PHE:CE1	1:B:94:MET:HE3	2.33	0.62
1:D:55:GLU:HB3	1:D:56:PRO:HD3	1.82	0.62
1:A:214:ILE:HG23	1:A:219:LEU:HD12	1.81	0.62
1:A:296:ASP:HA	5:A:743:HOH:O	2.00	0.62
1:D:126:VAL:HG11	1:D:141:PHE:CG	2.34	0.62
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.64	0.62
1:C:201:MET:HA	5:C:749:HOH:O	2.00	0.62
1:C:305:ARG:HB3	1:C:397:ILE:HD12	1.82	0.62
1:C:305:ARG:HB2	1:C:397:ILE:HG23	1.82	0.62
1:A:81:HIS:HE1	1:A:149:TRP:HB2	1.65	0.62
1:D:259:TYR:CE2	1:D:286:LEU:HD21	2.35	0.62
1:A:294:ARG:HH12	1:B:320:PRO:HB2	1.63	0.61
1:B:263:TRP:O	1:B:264:LEU:HB2	1.98	0.61
1:B:127:LYS:O	1:B:130:THR:CG2	2.48	0.61
1:D:116:TYR:O	1:D:117:SER:C	2.42	0.61
1:B:273:LEU:HD21	5:B:736:HOH:O	2.00	0.61
1:A:90:PHE:CE1	1:A:94:MET:HE3	2.36	0.61
1:B:347:TRP:CD1	1:B:348:GLY:N	2.67	0.61
1:B:369:GLU:HG3	1:B:370:PRO:CD	2.20	0.61
1:D:109:PHE:CZ	1:D:113:LYS:HE2	2.34	0.61
1:A:367:ILE:O	1:A:367:ILE:HD12	2.00	0.61
1:C:210:LYS:HE3	1:C:210:LYS:HA	1.81	0.61
1:B:210:LYS:HE2	1:B:213:GLU:OE2	2.01	0.61
1:C:156:TYR:CE2	1:C:219:LEU:HD22	2.36	0.61
1:C:237:GLY:O	1:C:241:GLU:HG3	2.01	0.60
1:D:43:VAL:HG22	1:D:47:THR:HG21	1.83	0.60
1:A:216:LYS:C	1:A:218:ASN:H	2.08	0.60
1:C:3:GLN:HE22	1:C:67:GLN:HE22	1.48	0.60
1:A:21:ILE:HD11	1:A:23:TYR:O	2.00	0.60
1:C:216:LYS:C	1:C:218:ASN:H	2.10	0.60
1:C:266:THR:HA	1:C:269:MET:HE3	1.83	0.60
1:C:234:LYS:HA	1:C:234:LYS:CE	2.30	0.60
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.67	0.60
1:D:171:GLN:NE2	1:D:230:ILE:H	1.90	0.60
1:A:333:ARG:NH1	1:A:363:LYS:HZ3	1.87	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLN:NE2	1:C:67:GLN:HE22	2.00	0.60
1:C:81:HIS:CD2	1:C:166:ASN:HD21	2.19	0.60
1:C:148:HIS:HD2	1:C:167:ASP:OD2	1.85	0.60
1:D:3:GLN:CD	1:D:67:GLN:HE22	2.10	0.60
1:A:72:VAL:CB	1:A:96:LEU:HD11	2.30	0.59
1:B:103:LEU:HD23	1:B:124:THR:HG23	1.84	0.59
1:B:308:LEU:N	1:B:308:LEU:HD23	2.17	0.59
1:B:372:PRO:CG	1:B:389:LEU:HD13	2.32	0.59
1:C:164:LEU:HD23	1:C:225:ALA:HB3	1.84	0.59
1:A:72:VAL:HB	1:A:96:LEU:CD1	2.32	0.59
1:A:81:HIS:CE1	1:A:149:TRP:HB2	2.38	0.59
1:C:327:ASP:OD2	1:D:358:ARG:NH2	2.36	0.59
1:A:372:PRO:HG3	1:A:389:LEU:CD1	2.32	0.59
1:C:40:TYR:CZ	1:C:225:ALA:HB1	2.38	0.59
1:C:200:LEU:O	5:C:749:HOH:O	2.16	0.58
1:C:320:PRO:CB	1:D:294:ARG:NH1	2.66	0.58
1:A:222:LYS:HB3	1:A:222:LYS:HZ1	1.67	0.58
1:A:320:PRO:CG	1:B:294:ARG:NH1	2.65	0.58
1:C:381:GLU:HG2	1:C:385:ARG:NH2	2.18	0.58
1:B:381:GLU:HG2	1:B:385:ARG:HH21	1.68	0.58
1:C:259:TYR:CE2	1:C:286:LEU:HD21	2.35	0.58
1:B:156:TYR:CZ	1:B:219:LEU:HD22	2.38	0.58
1:C:127:LYS:O	1:C:130:THR:CG2	2.52	0.58
1:B:107:ARG:HH11	1:B:107:ARG:CB	2.15	0.58
1:A:161:ALA:HB1	1:A:220:ALA:O	2.03	0.58
1:B:202:PRO:CG	1:B:332:LEU:HA	2.28	0.58
1:D:366:LEU:HD12	1:D:369:GLU:OE1	2.03	0.58
1:A:188:ILE:HG23	5:A:741:HOH:O	2.03	0.58
1:B:338:VAL:CG1	1:B:367:ILE:HD13	2.32	0.58
1:D:148:HIS:HD2	1:D:167:ASP:OD2	1.86	0.58
1:B:237:GLY:O	1:B:241:GLU:HG3	2.04	0.57
1:C:46:LYS:HA	1:C:75:ASP:OD2	2.04	0.57
1:C:82:THR:CG2	1:C:112:LEU:HD13	2.34	0.57
1:C:77:LEU:HD13	1:C:94:MET:HE1	1.85	0.57
1:D:213:GLU:HA	1:D:216:LYS:HE3	1.86	0.57
1:D:398:ALA:O	1:D:399:ASP:CB	2.52	0.57
1:D:109:PHE:CE2	1:D:113:LYS:CE	2.82	0.57
1:B:141:PHE:HD2	1:B:153:MET:CE	2.17	0.57
1:B:397:ILE:HD11	5:B:731:HOH:O	2.04	0.57
1:A:171:GLN:NE2	1:A:230:ILE:H	1.95	0.57
1:C:25:HIS:HB2	1:C:28:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ALA:O	1:C:399:ASP:CB	2.53	0.57
1:D:127:LYS:H	1:D:130:THR:HG21	1.69	0.57
1:B:117:SER:C	1:B:119:ILE:H	2.12	0.57
1:B:386:CYS:HA	5:B:736:HOH:O	2.04	0.57
1:B:177:VAL:HG22	1:B:182:GLN:CD	2.30	0.57
1:A:320:PRO:CB	1:B:294:ARG:NH1	2.68	0.56
1:C:177:VAL:HG22	1:C:182:GLN:OE1	2.05	0.56
1:A:98:PRO:HB2	1:D:279:ALA:O	2.05	0.56
1:A:163:LEU:HG	1:A:165:PRO:HG3	1.88	0.56
1:A:216:LYS:C	1:A:218:ASN:N	2.63	0.56
1:C:146:MET:C	1:C:148:HIS:N	2.63	0.56
1:C:184:ASP:OD2	1:C:187:LEU:HD13	2.05	0.56
1:D:224:ILE:HG13	1:D:236:PRO:HB3	1.87	0.56
1:B:261:THR:HG21	1:B:267:GLU:HB2	1.88	0.56
1:B:372:PRO:HG2	5:B:736:HOH:O	2.05	0.56
1:A:86:HIS:CE1	1:A:227:SER:HB2	2.40	0.56
1:D:391:ARG:HG3	1:D:391:ARG:HH11	1.71	0.56
1:A:55:GLU:HB3	1:A:56:PRO:HD3	1.87	0.56
1:A:359:LEU:HD22	1:A:364:ILE:HG21	1.86	0.56
1:B:81:HIS:HA	1:B:151:ASP:OD1	2.04	0.56
1:C:232:TRP:CZ2	1:C:239:ILE:HG13	2.41	0.56
1:C:4:PRO:HG3	1:C:64:LYS:HB3	1.87	0.56
1:D:117:SER:C	1:D:119:ILE:H	2.13	0.56
1:D:237:GLY:O	1:D:241:GLU:HG3	2.06	0.56
1:D:232:TRP:CZ2	1:D:239:ILE:HG13	2.41	0.56
1:C:216:LYS:C	1:C:218:ASN:N	2.63	0.56
1:A:117:SER:C	1:A:119:ILE:H	2.14	0.55
1:B:13:TRP:NE1	1:B:38:ASN:OD1	2.31	0.55
1:A:306:ALA:CB	1:A:397:ILE:HD11	2.37	0.55
1:B:216:LYS:C	1:B:218:ASN:H	2.15	0.55
1:C:333:ARG:HG2	5:C:802:HOH:O	2.06	0.55
1:D:266:THR:HA	1:D:269:MET:HE3	1.88	0.55
1:B:69:LYS:NZ	5:B:756:HOH:O	2.35	0.55
1:B:206:LEU:HB2	5:B:753:HOH:O	2.06	0.55
1:C:372:PRO:HG3	1:C:389:LEU:CD1	2.36	0.55
1:D:164:LEU:HD23	1:D:225:ALA:HB3	1.88	0.55
1:B:379:ARG:HG3	1:B:382:ASP:OD2	2.07	0.55
1:C:185:ALA:HB1	1:C:238:ARG:NH1	2.22	0.55
1:A:139:LEU:HD13	1:A:141:PHE:HZ	1.72	0.54
1:B:146:MET:C	1:B:148:HIS:N	2.65	0.54
1:A:187:LEU:N	1:A:187:LEU:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:O	1:D:67:GLN:HG3	2.07	0.54
1:C:372:PRO:CG	1:C:389:LEU:HD12	2.35	0.54
1:A:306:ALA:HB2	1:A:397:ILE:HD11	1.88	0.54
1:D:216:LYS:C	1:D:218:ASN:H	2.15	0.54
1:A:146:MET:C	1:A:148:HIS:N	2.62	0.54
1:A:263:TRP:O	1:A:264:LEU:CB	2.56	0.54
1:C:126:VAL:HG13	1:C:130:THR:CG2	2.36	0.54
1:D:146:MET:C	1:D:148:HIS:N	2.63	0.54
1:D:321:VAL:HG23	5:D:734:HOH:O	2.08	0.54
1:C:259:TYR:HE2	1:C:286:LEU:CD2	2.20	0.54
1:D:127:LYS:H	1:D:130:THR:HG23	1.70	0.54
1:B:134:LEU:HG	5:B:752:HOH:O	2.07	0.54
1:C:212:ASP:O	1:C:215:GLN:HB3	2.07	0.54
1:D:72:VAL:HB	1:D:96:LEU:CD1	2.37	0.54
1:C:76:TYR:CD1	1:C:101:HIS:HB3	2.43	0.54
1:C:117:SER:C	1:C:119:ILE:H	2.15	0.54
1:B:159:GLU:N	5:B:766:HOH:O	2.40	0.53
1:B:365:GLU:CD	1:B:396:ARG:HH22	2.16	0.53
1:C:116:TYR:O	1:C:117:SER:C	2.51	0.53
1:B:299:LYS:HE3	5:B:750:HOH:O	2.08	0.53
1:D:261:THR:HG21	1:D:267:GLU:H	1.72	0.53
1:A:379:ARG:NH1	1:A:382:ASP:OD1	2.41	0.53
1:B:144:ALA:N	1:B:145:PRO:HD3	2.24	0.53
1:A:171:GLN:HE22	1:A:230:ILE:N	1.96	0.53
1:A:261:THR:HG21	1:A:267:GLU:H	1.74	0.53
1:D:116:TYR:C	1:D:117:SER:O	2.52	0.53
1:A:217:ILE:O	1:A:217:ILE:HG22	2.09	0.53
1:B:395:ALA:O	1:B:398:ALA:HB2	2.08	0.53
1:A:365:GLU:CD	1:A:396:ARG:HH22	2.17	0.53
1:B:70:ASP:C	5:B:756:HOH:O	2.51	0.53
1:B:274:MET:HG3	1:B:284:VAL:HG11	1.91	0.53
1:C:367:ILE:O	1:C:367:ILE:HG13	2.08	0.53
1:B:194:LYS:HG3	5:B:750:HOH:O	2.09	0.52
1:D:46:LYS:HA	1:D:75:ASP:OD2	2.09	0.52
1:A:206:LEU:HB3	5:A:757:HOH:O	2.10	0.52
1:A:291:VAL:O	1:A:291:VAL:CG1	2.58	0.52
1:B:279:ALA:HB3	5:B:713:HOH:O	2.08	0.52
1:D:109:PHE:HE2	1:D:113:LYS:HE2	1.66	0.52
1:A:21:ILE:HG23	1:A:34:GLY:HA2	1.91	0.52
1:B:137:ARG:HA	1:B:159:GLU:CD	2.34	0.52
1:C:323:SER:HB2	1:C:324:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:CD1	1:D:284:VAL:HG13	2.40	0.52
1:C:308:LEU:N	1:C:308:LEU:HD23	2.25	0.52
1:C:358:ARG:HD2	5:C:786:HOH:O	2.10	0.52
1:D:73:LYS:CG	1:D:73:LYS:O	2.58	0.52
1:C:149:TRP:HB2	5:C:745:HOH:O	2.09	0.52
1:A:323:SER:HB3	1:B:323:SER:HB3	1.91	0.52
1:C:126:VAL:HG11	1:C:141:PHE:CG	2.45	0.52
1:B:338:VAL:HB	5:B:731:HOH:O	2.09	0.52
1:C:77:LEU:CD1	1:C:94:MET:HE1	2.40	0.51
1:C:189:MET:HE3	1:C:238:ARG:NE	2.24	0.51
1:A:134:LEU:HG	5:A:754:HOH:O	2.10	0.51
1:A:259:TYR:HE2	1:A:286:LEU:HD21	1.74	0.51
1:A:379:ARG:HG2	1:A:382:ASP:OD2	2.10	0.51
1:B:147:LEU:CD1	5:B:753:HOH:O	2.49	0.51
1:D:107:ARG:HG2	5:D:751:HOH:O	2.10	0.51
1:B:116:TYR:O	1:B:117:SER:C	2.54	0.51
1:B:291:VAL:HG13	1:B:291:VAL:O	2.10	0.51
1:B:381:GLU:HG2	1:B:385:ARG:NH2	2.25	0.51
1:B:216:LYS:C	1:B:218:ASN:N	2.67	0.51
1:C:38:ASN:HB2	1:C:227:SER:HA	1.92	0.51
1:C:80:ASN:ND2	1:C:153:MET:HE3	2.25	0.51
1:A:118:HIS:HD1	1:D:388:GLU:CD	2.18	0.51
1:B:262:MET:HE1	4:B:711:FMN:HM83	1.91	0.51
1:B:101:HIS:CD2	1:B:124:THR:HG22	2.45	0.51
1:A:341:ALA:C	1:A:352:GLN:HE22	2.19	0.51
1:B:80:ASN:HD22	1:B:153:MET:HG3	1.75	0.51
1:D:216:LYS:C	1:D:218:ASN:N	2.67	0.51
1:B:141:PHE:CB	1:B:153:MET:HE1	2.41	0.51
1:B:305:ARG:HB2	1:B:397:ILE:CG2	2.40	0.51
1:C:161:ALA:HB3	1:C:222:LYS:HB2	1.92	0.51
1:D:262:MET:CE	1:D:314:ILE:HD12	2.40	0.51
1:B:291:VAL:O	1:B:291:VAL:CG1	2.59	0.50
1:A:126:VAL:HG13	1:A:130:THR:CG2	2.42	0.50
1:C:323:SER:HB3	1:D:323:SER:HB3	1.93	0.50
1:D:397:ILE:O	1:D:397:ILE:HG22	2.11	0.50
1:B:90:PHE:HB3	1:B:91:PRO:HD3	1.93	0.50
1:B:189:MET:HE3	1:B:238:ARG:HD3	1.92	0.50
1:C:312:PRO:CD	1:C:319:LEU:HD22	2.42	0.50
1:A:72:VAL:HG13	1:A:74:LEU:HD13	1.93	0.50
1:C:327:ASP:HA	5:C:786:HOH:O	2.11	0.50
1:D:215:GLN:OE1	1:D:215:GLN:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TYR:CZ	1:B:225:ALA:HB1	2.47	0.50
1:C:307:VAL:C	1:C:308:LEU:HD23	2.37	0.50
1:C:347:TRP:CD1	1:C:348:GLY:H	2.29	0.50
1:D:21:ILE:HG23	1:D:34:GLY:HA2	1.94	0.50
1:A:301:ILE:O	1:A:337:LYS:HE3	2.11	0.50
1:D:40:TYR:CZ	1:D:225:ALA:HB1	2.47	0.50
1:D:217:ILE:O	1:D:217:ILE:HG22	2.12	0.50
1:A:59:GLU:CD	1:A:59:GLU:H	2.20	0.50
1:A:128:THR:N	1:A:143:GLU:HG3	2.27	0.50
1:A:390:GLY:HA3	5:A:765:HOH:O	2.12	0.50
1:D:72:VAL:HB	1:D:96:LEU:HD11	1.93	0.50
1:A:259:TYR:OH	1:A:267:GLU:OE1	2.24	0.49
1:B:336:ASN:CG	1:B:336:ASN:O	2.55	0.49
1:C:336:ASN:CG	1:C:336:ASN:O	2.55	0.49
1:A:313:THR:HG22	1:A:351:ALA:CB	2.42	0.49
1:A:345:TYR:HE2	1:A:373:THR:HG23	1.75	0.49
1:B:214:ILE:HG23	1:B:219:LEU:HD12	1.94	0.49
1:B:389:LEU:O	1:B:393:ILE:HG13	2.11	0.49
1:A:127:LYS:H	1:A:130:THR:HG23	1.77	0.49
1:B:144:ALA:N	1:B:145:PRO:CD	2.75	0.49
1:B:323:SER:HB2	1:B:324:PRO:HD3	1.94	0.49
1:C:372:PRO:CG	1:C:389:LEU:CD1	2.90	0.49
1:A:259:TYR:CE2	1:A:286:LEU:HD21	2.48	0.49
1:C:369:GLU:CG	1:C:370:PRO:HD3	2.40	0.49
1:D:131:SER:OG	1:D:140:THR:HB	2.13	0.49
1:A:314:ILE:HD11	1:A:318:ILE:C	2.37	0.49
1:B:202:PRO:HG3	1:B:332:LEU:C	2.37	0.49
1:A:235:ASP:OD1	1:A:238:ARG:HG3	2.12	0.49
1:B:201:MET:HB3	1:B:202:PRO:HD3	1.94	0.49
1:D:73:LYS:O	1:D:73:LYS:HG3	2.13	0.49
1:D:372:PRO:CG	1:D:389:LEU:CD1	2.90	0.49
1:A:126:VAL:HG11	1:A:141:PHE:CD1	2.47	0.49
1:D:117:SER:C	1:D:119:ILE:N	2.71	0.49
1:A:126:VAL:HG13	1:A:130:THR:OG1	2.12	0.48
1:A:210:LYS:HE3	1:A:210:LYS:HA	1.95	0.48
1:C:31:THR:HG22	1:C:172:HIS:HB3	1.94	0.48
1:D:194:LYS:HB2	1:D:299:LYS:HD3	1.95	0.48
1:A:314:ILE:HD11	1:A:319:LEU:N	2.28	0.48
1:A:314:ILE:CD1	1:A:319:LEU:HA	2.32	0.48
1:B:157:VAL:HG12	1:B:157:VAL:O	2.12	0.48
1:A:333:ARG:HD2	1:A:363:LYS:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:PRO:HD2	1:D:319:LEU:HD22	1.94	0.48
1:A:203:PHE:HB3	1:A:206:LEU:HD12	1.96	0.48
1:A:314:ILE:HG12	1:A:319:LEU:CD1	2.42	0.48
1:B:3:GLN:HG2	5:B:733:HOH:O	2.11	0.48
1:C:222:LYS:HE2	5:C:804:HOH:O	2.14	0.48
1:C:254:LYS:HG2	1:C:255:ALA:N	2.28	0.48
1:D:159:GLU:H	1:D:159:GLU:CD	2.21	0.48
1:D:323:SER:HB2	1:D:324:PRO:HD3	1.96	0.48
1:A:314:ILE:CD1	1:A:318:ILE:O	2.62	0.48
1:B:161:ALA:HB1	1:B:220:ALA:O	2.14	0.48
1:D:396:ARG:C	1:D:398:ALA:H	2.21	0.48
1:B:86:HIS:CE1	1:B:227:SER:HB2	2.49	0.48
1:C:398:ALA:O	1:C:399:ASP:HB3	2.14	0.48
1:C:116:TYR:C	1:C:117:SER:O	2.56	0.48
1:C:305:ARG:CB	1:C:397:ILE:HD12	2.43	0.48
1:D:347:TRP:CD1	1:D:348:GLY:H	2.31	0.48
1:A:80:ASN:HD22	1:A:153:MET:HG3	1.78	0.47
1:B:90:PHE:CE1	1:B:94:MET:HE2	2.48	0.47
1:B:117:SER:C	1:B:119:ILE:N	2.70	0.47
1:B:46:LYS:CA	1:B:75:ASP:OD2	2.60	0.47
1:C:137:ARG:HG3	1:C:137:ARG:NH1	2.28	0.47
1:C:294:ARG:NH1	1:D:320:PRO:HG2	2.27	0.47
1:D:288:LYS:HE3	5:D:795:HOH:O	2.14	0.47
1:A:99:ASP:OD1	1:A:99:ASP:N	2.46	0.47
1:D:83:GLU:HG2	1:D:149:TRP:CH2	2.49	0.47
1:A:177:VAL:CG1	1:A:182:GLN:HB2	2.45	0.47
1:A:397:ILE:O	1:A:397:ILE:HG22	2.14	0.47
1:B:38:ASN:HB2	1:B:227:SER:HA	1.96	0.47
1:B:216:LYS:O	1:B:218:ASN:N	2.47	0.47
1:B:306:ALA:HB2	5:B:731:HOH:O	2.14	0.47
1:D:30:SER:H	1:D:295:ASN:ND2	2.11	0.47
1:D:86:HIS:CD2	5:D:760:HOH:O	2.66	0.47
1:B:73:LYS:HD3	1:B:75:ASP:OD1	2.15	0.47
1:D:166:ASN:ND2	1:D:167:ASP:H	2.12	0.47
1:A:117:SER:C	1:A:119:ILE:N	2.71	0.47
1:A:314:ILE:HG12	1:A:319:LEU:HD13	1.97	0.47
1:A:365:GLU:OE2	1:A:396:ARG:NH2	2.47	0.47
1:B:112:LEU:HB3	5:B:740:HOH:O	2.14	0.47
1:B:263:TRP:O	1:B:264:LEU:CB	2.63	0.47
1:B:286:LEU:HD23	1:B:286:LEU:C	2.39	0.47
1:C:201:MET:N	1:C:202:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:GLU:HG2	1:D:366:LEU:HD13	1.97	0.47
1:A:212:ASP:O	1:A:215:GLN:HB3	2.15	0.47
1:C:258:ALA:HB1	1:C:289:LEU:HD21	1.97	0.47
1:A:159:GLU:CD	1:A:159:GLU:N	2.70	0.47
1:C:27:PRO:CB	1:D:321:VAL:HG21	2.46	0.46
1:D:8:THR:HG23	1:D:11:ILE:CD1	2.45	0.46
1:D:90:PHE:HB3	1:D:91:PRO:HD3	1.97	0.46
1:D:112:LEU:HD12	1:D:112:LEU:HA	1.80	0.46
1:D:116:TYR:O	1:D:117:SER:O	2.32	0.46
1:B:212:ASP:O	1:B:215:GLN:HB3	2.15	0.46
1:B:144:ALA:HB1	1:B:147:LEU:HB2	1.96	0.46
1:D:108:ALA:HB2	1:D:151:ASP:HB2	1.96	0.46
1:D:215:GLN:HG2	5:D:757:HOH:O	2.16	0.46
1:C:320:PRO:HG2	1:D:294:ARG:HH12	1.79	0.46
1:D:286:LEU:C	1:D:286:LEU:HD23	2.41	0.46
1:D:375:GLN:O	1:D:376:TRP:HB2	2.16	0.46
1:B:109:PHE:CZ	1:B:123:TYR:CZ	3.03	0.46
1:B:305:ARG:HD2	1:B:397:ILE:HG23	1.98	0.46
1:D:73:LYS:HB2	1:D:73:LYS:NZ	2.30	0.46
1:B:12:TYR:CE2	1:B:68:ILE:HD12	2.51	0.46
1:D:67:GLN:HE21	1:D:67:GLN:HB3	1.57	0.46
1:D:232:TRP:O	1:D:236:PRO:HG3	2.15	0.46
1:B:13:TRP:CZ3	1:B:64:LYS:HE2	2.51	0.46
1:D:259:TYR:HE2	1:D:286:LEU:CD2	2.25	0.46
1:A:177:VAL:HG11	1:A:182:GLN:HB2	1.98	0.46
1:C:177:VAL:HG22	1:C:182:GLN:CD	2.41	0.46
1:D:254:LYS:HG2	1:D:255:ALA:N	2.31	0.46
1:D:294:ARG:HE	1:D:294:ARG:HB3	1.39	0.46
1:A:25:HIS:HB2	1:A:28:ALA:HB3	1.97	0.46
1:A:213:GLU:O	1:A:217:ILE:HG13	2.16	0.46
1:C:216:LYS:O	1:C:218:ASN:N	2.49	0.46
1:C:396:ARG:C	1:C:398:ALA:H	2.23	0.46
1:A:164:LEU:HD23	1:A:225:ALA:HB3	1.97	0.45
1:C:21:ILE:HG21	1:C:35:THR:HG22	1.97	0.45
1:D:58:LYS:O	1:D:62:ILE:HG13	2.16	0.45
1:D:147:LEU:HA	1:D:147:LEU:HD12	1.37	0.45
1:A:273:LEU:HA	5:A:765:HOH:O	2.15	0.45
1:C:47:THR:HG23	5:C:766:HOH:O	2.15	0.45
1:C:81:HIS:CB	1:C:166:ASN:ND2	2.79	0.45
1:A:162:LEU:HA	1:A:223:THR:HG23	1.99	0.45
1:B:77:LEU:CD1	1:B:94:MET:HE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:THR:CG2	1:B:351:ALA:H	2.29	0.45
1:B:156:TYR:CZ	1:B:219:LEU:CD2	3.00	0.45
1:D:263:TRP:O	1:D:264:LEU:HB2	2.17	0.45
1:A:142:ILE:HD11	1:A:219:LEU:HD11	1.99	0.45
1:A:308:LEU:CD2	1:A:308:LEU:N	2.80	0.45
1:D:83:GLU:C	5:D:760:HOH:O	2.60	0.45
1:D:311:SER:HA	1:D:312:PRO:HD3	1.82	0.45
1:B:93:ILE:HD13	1:B:93:ILE:HA	1.85	0.45
1:C:156:TYR:CZ	1:C:219:LEU:HD22	2.51	0.45
1:C:381:GLU:H	1:C:381:GLU:CD	2.18	0.45
1:A:294:ARG:NH1	1:B:320:PRO:CB	2.74	0.45
1:A:315:ASN:HA	5:A:742:HOH:O	2.17	0.45
1:B:55:GLU:HB3	1:B:56:PRO:HD3	1.98	0.45
1:B:141:PHE:CD2	1:B:153:MET:CE	2.93	0.45
1:C:345:TYR:HA	4:C:721:FMN:O2'	2.17	0.45
1:A:126:VAL:HG12	1:A:127:LYS:N	2.30	0.45
1:B:81:HIS:HE1	1:B:149:TRP:CG	2.35	0.45
1:B:305:ARG:HH12	1:B:399:ASP:HB2	1.82	0.45
1:C:3:GLN:CD	1:C:67:GLN:HE22	2.25	0.45
1:C:116:TYR:O	1:C:117:SER:O	2.34	0.45
1:D:86:HIS:N	5:D:760:HOH:O	2.45	0.45
1:C:82:THR:C	1:C:83:GLU:O	2.58	0.44
1:B:341:ALA:HB3	1:B:352:GLN:NE2	2.33	0.44
1:C:238:ARG:HD3	5:C:805:HOH:O	2.18	0.44
1:A:116:TYR:O	1:A:117:SER:C	2.60	0.44
1:A:184:ASP:CG	1:A:187:LEU:HD13	2.43	0.44
1:A:387:TYR:HA	5:A:765:HOH:O	2.18	0.44
1:B:35:THR:OG1	1:B:36:THR:N	2.51	0.44
1:B:108:ALA:CA	1:B:151:ASP:HB2	2.48	0.44
1:D:21:ILE:HG21	1:D:35:THR:HG22	1.99	0.44
1:A:73:LYS:HE2	1:A:73:LYS:O	2.17	0.44
1:A:103:LEU:HD23	1:A:124:THR:HG23	2.00	0.44
1:A:203:PHE:O	1:A:207:ILE:HG12	2.17	0.44
1:B:397:ILE:HG22	1:B:397:ILE:O	2.18	0.44
1:C:27:PRO:HB2	1:D:321:VAL:HG21	1.99	0.44
1:A:286:LEU:HG	5:A:746:HOH:O	2.16	0.44
1:B:86:HIS:CE1	1:B:228:HIS:CE1	3.06	0.44
1:B:398:ALA:O	1:B:399:ASP:CB	2.65	0.44
1:C:306:ALA:HA	1:C:338:VAL:O	2.17	0.44
1:A:261:THR:HG21	1:A:267:GLU:N	2.33	0.44
1:C:311:SER:HA	1:C:312:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ILE:HD13	1:D:319:LEU:O	2.17	0.44
1:B:77:LEU:HD12	1:B:94:MET:HE1	1.99	0.44
1:B:164:LEU:HD23	1:B:225:ALA:HB3	2.00	0.44
1:B:367:ILE:HD11	1:B:396:ARG:HD3	2.00	0.44
1:D:3:GLN:NE2	1:D:67:GLN:HE22	2.15	0.44
1:D:95:GLU:O	1:D:95:GLU:HG2	2.18	0.44
1:B:121:PHE:HZ	5:B:740:HOH:O	2.01	0.43
1:C:44:ASP:H	1:C:47:THR:HG22	1.83	0.43
1:A:165:PRO:O	1:A:166:ASN:HB3	2.17	0.43
1:A:320:PRO:CB	1:B:294:ARG:HH11	2.31	0.43
1:A:398:ALA:O	1:A:399:ASP:HB2	2.17	0.43
1:C:117:SER:C	1:C:119:ILE:N	2.76	0.43
1:C:222:LYS:O	1:C:223:THR:HG22	2.17	0.43
1:D:286:LEU:HD23	1:D:287:PHE:N	2.32	0.43
1:A:134:LEU:HD11	1:A:139:LEU:HD23	2.01	0.43
1:A:216:LYS:O	1:A:218:ASN:N	2.52	0.43
1:B:54:TYR:CD2	1:B:56:PRO:HD2	2.53	0.43
1:B:366:LEU:N	1:B:366:LEU:HD23	2.33	0.43
1:B:393:ILE:O	1:B:397:ILE:HG12	2.19	0.43
1:D:14:VAL:HG11	5:D:796:HOH:O	2.18	0.43
1:A:139:LEU:CD1	1:A:141:PHE:CZ	3.01	0.43
1:D:81:HIS:NE2	1:D:83:GLU:HG3	2.33	0.43
1:D:177:VAL:HG22	1:D:182:GLN:CD	2.43	0.43
1:D:301:ILE:O	1:D:337:LYS:HE3	2.18	0.43
1:B:81:HIS:CE1	1:B:149:TRP:HB2	2.54	0.43
1:B:375:GLN:O	1:B:376:TRP:HB2	2.18	0.43
1:A:72:VAL:HG12	1:A:74:LEU:HD13	1.96	0.43
1:A:81:HIS:CD2	1:A:166:ASN:HD21	2.36	0.43
1:B:25:HIS:CB	1:B:28:ALA:HB3	2.48	0.43
1:B:139:LEU:HD13	1:B:141:PHE:CZ	2.53	0.43
1:B:254:LYS:HG3	1:B:283:GLU:HG2	2.01	0.43
1:B:396:ARG:C	1:B:398:ALA:H	2.26	0.43
1:D:324:PRO:O	1:D:328:ASP:HB2	2.18	0.43
1:B:314:ILE:HD11	1:B:319:LEU:N	2.32	0.43
1:B:366:LEU:HB3	5:B:729:HOH:O	2.19	0.43
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.49	0.43
1:B:3:GLN:HA	1:B:4:PRO:HD3	1.84	0.43
1:B:50:VAL:HG23	5:B:765:HOH:O	2.18	0.43
1:B:116:TYR:C	1:B:117:SER:O	2.62	0.43
1:A:128:THR:HG23	1:A:142:ILE:HA	2.01	0.43
1:B:328:ASP:O	1:B:332:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:SER:HB2	1:C:140:THR:HB	2.01	0.43
1:D:263:TRP:O	1:D:264:LEU:CB	2.67	0.43
1:A:201:MET:N	1:A:202:PRO:CD	2.82	0.43
1:A:379:ARG:NH1	1:A:382:ASP:CG	2.74	0.43
1:B:24:PHE:HB3	1:B:29:PHE:HB3	2.01	0.43
1:A:50:VAL:HG21	1:A:164:LEU:CD1	2.49	0.42
1:A:291:VAL:O	1:A:291:VAL:HG13	2.19	0.42
1:B:188:ILE:HD12	1:B:188:ILE:HA	1.91	0.42
1:B:222:LYS:O	1:B:223:THR:HG22	2.19	0.42
1:D:14:VAL:O	1:D:14:VAL:HG23	2.19	0.42
1:D:24:PHE:HZ	1:D:85:ASP:HB3	1.84	0.42
1:D:31:THR:HG22	1:D:172:HIS:HB3	2.00	0.42
1:D:166:ASN:HD22	1:D:167:ASP:H	1.65	0.42
1:B:70:ASP:OD1	1:B:71:PRO:CD	2.66	0.42
1:B:194:LYS:HB2	1:B:299:LYS:HD3	2.00	0.42
1:C:137:ARG:HD3	1:C:159:GLU:HB2	2.01	0.42
1:C:277:LEU:O	1:C:282:CYS:HB2	2.20	0.42
1:D:232:TRP:CZ2	1:D:239:ILE:CG1	3.02	0.42
1:D:254:LYS:NZ	1:D:300:GLU:OE1	2.50	0.42
1:A:127:LYS:O	1:A:130:THR:CG2	2.58	0.42
1:A:27:PRO:HG2	1:B:321:VAL:HG21	1.99	0.42
1:C:73:LYS:HE2	1:C:73:LYS:HA	2.00	0.42
1:C:393:ILE:O	1:C:397:ILE:HG12	2.19	0.42
1:D:70:ASP:OD1	1:D:70:ASP:C	2.62	0.42
1:A:156:TYR:CZ	1:A:219:LEU:HD22	2.55	0.42
1:A:375:GLN:O	1:A:376:TRP:HB2	2.19	0.42
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.84	0.42
1:C:294:ARG:HE	1:C:294:ARG:HB3	1.48	0.42
1:A:168:ALA:O	1:A:169:PHE:HB2	2.19	0.42
1:C:21:ILE:CG2	1:C:34:GLY:HA2	2.50	0.42
1:A:144:ALA:N	1:A:145:PRO:HD3	2.35	0.42
1:A:208:THR:HG22	5:A:704:HOH:O	2.19	0.42
1:D:168:ALA:O	1:D:169:PHE:HB2	2.18	0.42
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.20	0.42
1:D:321:VAL:O	1:D:321:VAL:HG12	2.20	0.42
1:A:53:VAL:HB	1:A:61:LEU:HD22	2.01	0.42
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.80	0.42
1:D:82:THR:C	1:D:83:GLU:O	2.61	0.42
1:A:233:ARG:O	1:A:233:ARG:HG2	2.12	0.42
1:A:368:ALA:O	1:A:369:GLU:C	2.61	0.42
1:D:125:ILE:N	1:D:125:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:TYR:CD1	1:D:260:ASP:N	2.88	0.42
1:D:396:ARG:C	1:D:398:ALA:N	2.78	0.42
1:A:222:LYS:NZ	1:A:222:LYS:CB	2.79	0.42
1:A:13:TRP:CZ3	1:A:64:LYS:HE2	2.55	0.41
1:A:205:ASN:HB2	5:A:756:HOH:O	2.19	0.41
1:B:107:ARG:HH11	1:B:107:ARG:HA	1.85	0.41
1:B:379:ARG:CB	1:B:381:GLU:OE2	2.60	0.41
1:C:396:ARG:C	1:C:398:ALA:N	2.77	0.41
1:D:117:SER:HB2	1:D:118:HIS:H	1.70	0.41
1:D:173:ILE:C	1:D:173:ILE:HD13	2.44	0.41
1:C:60:GLU:OE1	1:C:64:LYS:NZ	2.53	0.41
1:C:217:ILE:HD11	5:C:737:HOH:O	2.19	0.41
1:D:52:THR:OG1	1:D:53:VAL:N	2.52	0.41
1:A:30:SER:H	1:A:295:ASN:ND2	2.17	0.41
1:A:101:HIS:NE2	1:A:124:THR:HG22	2.35	0.41
1:B:205:ASN:O	1:B:209:LYS:HG3	2.20	0.41
1:A:245:ARG:HE	1:A:245:ARG:HB3	1.63	0.41
1:A:252:LYS:O	1:A:254:LYS:N	2.50	0.41
1:C:144:ALA:HB1	1:C:147:LEU:HB2	2.03	0.41
1:A:117:SER:O	1:A:118:HIS:C	2.58	0.41
1:A:333:ARG:HA	1:A:333:ARG:HD3	1.89	0.41
1:C:211:LEU:HD23	1:C:211:LEU:HA	1.78	0.41
1:D:313:THR:HG21	1:D:349:GLY:HA2	2.03	0.41
1:D:398:ALA:O	1:D:399:ASP:HB3	2.19	0.41
1:B:107:ARG:NH1	1:B:107:ARG:CB	2.74	0.41
1:C:21:ILE:HG22	1:C:34:GLY:HA2	2.01	0.41
1:C:294:ARG:NH1	1:D:320:PRO:CB	2.83	0.41
1:D:306:ALA:HB3	1:D:397:ILE:HD11	2.01	0.41
1:D:376:TRP:HA	1:D:376:TRP:CE3	2.56	0.41
1:A:276:GLY:HA3	5:A:765:HOH:O	2.20	0.41
1:B:52:THR:OG1	1:B:86:HIS:O	2.32	0.41
1:B:326:LEU:HD11	1:B:355:LEU:HD23	2.01	0.41
1:B:398:ALA:O	1:B:399:ASP:HB3	2.21	0.41
1:C:86:HIS:CE1	1:C:227:SER:HB2	2.56	0.41
1:D:318:ILE:HD13	1:D:322:VAL:HB	1.96	0.41
1:A:21:ILE:CG2	1:A:34:GLY:HA2	2.50	0.41
1:A:187:LEU:N	1:A:187:LEU:CD1	2.83	0.41
1:A:188:ILE:HD12	1:A:188:ILE:HA	1.87	0.41
1:B:368:ALA:O	1:B:369:GLU:C	2.63	0.41
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.81	0.41
1:A:320:PRO:HB2	1:B:294:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:HG22	1:B:172:HIS:HB3	2.01	0.41
1:C:50:VAL:HA	1:C:78:VAL:HB	2.03	0.41
1:C:389:LEU:HA	1:C:389:LEU:HD23	1.86	0.41
1:D:183:VAL:HG12	1:D:184:ASP:N	2.36	0.41
1:A:206:LEU:HG	5:A:756:HOH:O	2.21	0.41
1:B:356:GLU:HG2	1:B:366:LEU:HD11	1.98	0.41
1:D:379:ARG:O	1:D:382:ASP:HB2	2.21	0.41
1:A:156:TYR:CE2	1:A:219:LEU:CD2	3.04	0.40
1:B:367:ILE:CD1	1:B:396:ARG:HH11	2.34	0.40
1:D:391:ARG:NH1	1:D:391:ARG:CG	2.82	0.40
1:A:109:PHE:O	1:A:113:LYS:HG2	2.20	0.40
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.88	0.40
1:A:398:ALA:O	1:A:399:ASP:HB3	2.17	0.40
1:B:165:PRO:O	1:B:166:ASN:HB3	2.21	0.40
1:C:159:GLU:H	1:C:159:GLU:CD	2.29	0.40
1:C:189:MET:HE3	1:C:238:ARG:CZ	2.50	0.40
1:D:188:ILE:HD13	1:D:230:ILE:HG21	2.03	0.40
1:A:356:GLU:HG2	1:A:366:LEU:HD13	2.03	0.40
1:A:397:ILE:HG21	1:A:397:ILE:HD13	1.80	0.40
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.33	0.40
1:D:3:GLN:HA	1:D:4:PRO:HD3	1.93	0.40
1:A:325:LEU:O	1:A:329:LEU:HG	2.21	0.40
1:B:141:PHE:CG	1:B:153:MET:HE1	2.57	0.40
1:C:26:GLY:HA3	1:C:27:PRO:HD3	1.78	0.40
1:C:80:ASN:HD22	1:C:153:MET:HE3	1.87	0.40
1:A:237:GLY:O	1:A:241:GLU:HG3	2.22	0.40
1:B:47:THR:N	1:B:75:ASP:OD2	2.55	0.40
1:B:147:LEU:HA	1:B:147:LEU:HD12	1.39	0.40
1:C:232:TRP:CZ2	1:C:239:ILE:CG1	3.04	0.40
1:D:38:ASN:HB2	1:D:227:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/398 (100%)	360 (91%)	26 (7%)	10 (2%)	4	16
1	B	396/398 (100%)	359 (91%)	28 (7%)	9 (2%)	5	18
1	C	396/398 (100%)	365 (92%)	23 (6%)	8 (2%)	6	21
1	D	396/398 (100%)	362 (91%)	26 (7%)	8 (2%)	6	21
All	All	1584/1592 (100%)	1446 (91%)	103 (6%)	35 (2%)	5	19

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	118	HIS
1	A	148	HIS
1	A	370	PRO
1	A	398	ALA
1	B	71	PRO
1	B	118	HIS
1	B	148	HIS
1	B	370	PRO
1	B	398	ALA
1	C	118	HIS
1	C	148	HIS
1	C	370	PRO
1	C	398	ALA
1	D	118	HIS
1	D	148	HIS
1	D	370	PRO
1	D	398	ALA
1	B	117	SER
1	C	74	LEU
1	C	117	SER
1	D	117	SER
1	A	74	LEU
1	B	74	LEU
1	A	368	ALA
1	A	376	TRP
1	B	217	ILE
1	B	376	TRP
1	C	376	TRP
1	D	368	ALA

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Mol	Chain	Res	Type
1	D	376	TRP
1	A	117	SER
1	C	217	ILE
1	A	217	ILE
1	D	71	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	329/329 (100%)	288 (88%)	41 (12%)	4 15
1	B	329/329 (100%)	297 (90%)	32 (10%)	8 25
1	C	329/329 (100%)	301 (92%)	28 (8%)	10 31
1	D	329/329 (100%)	287 (87%)	42 (13%)	4 15
All	All	1316/1316 (100%)	1173 (89%)	143 (11%)	6 21

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	53	VAL
1	A	71	PRO
1	A	73	LYS
1	A	77	LEU
1	A	84	SER
1	A	96	LEU
1	A	112	LEU
1	A	124	THR
1	A	130	THR
1	A	139	LEU
1	A	140	THR
1	A	147	LEU
1	A	162	LEU
1	A	171	GLN
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	204	SER
1	A	208	THR
1	A	210	LYS
1	A	222	LYS
1	A	230	ILE
1	A	233	ARG
1	A	234	LYS
1	A	239	ILE
1	A	282	CYS
1	A	291	VAL
1	A	308	LEU
1	A	313	THR
1	A	314	ILE
1	A	321	VAL
1	A	325	LEU
1	A	360	LYS
1	A	363	LYS
1	A	364	ILE
1	A	367	ILE
1	A	373	THR
1	A	377	VAL
1	A	379	ARG
1	A	381	GLU
1	A	389	LEU
1	A	391	ARG
1	B	53	VAL
1	B	71	PRO
1	B	73	LYS
1	B	77	LEU
1	B	93	ILE
1	B	107	ARG
1	B	124	THR
1	B	130	THR
1	B	139	LEU
1	B	140	THR
1	B	147	LEU
1	B	150	PRO
1	B	162	LEU
1	B	171	GLN
1	B	177	VAL
1	B	210	LYS
1	B	218	ASN

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Mol	Chain	Res	Type
1	B	223	THR
1	B	230	ILE
1	B	233	ARG
1	B	239	ILE
1	B	261	THR
1	B	291	VAL
1	B	308	LEU
1	B	313	THR
1	B	314	ILE
1	B	321	VAL
1	B	325	LEU
1	B	370	PRO
1	B	374	VAL
1	B	379	ARG
1	B	381	GLU
1	C	53	VAL
1	C	73	LYS
1	C	96	LEU
1	C	112	LEU
1	C	122	ASN
1	C	127	LYS
1	C	130	THR
1	C	131	SER
1	C	137	ARG
1	C	140	THR
1	C	147	LEU
1	C	162	LEU
1	C	208	THR
1	C	210	LYS
1	C	222	LYS
1	C	230	ILE
1	C	234	LYS
1	C	239	ILE
1	C	261	THR
1	C	282	CYS
1	C	291	VAL
1	C	308	LEU
1	C	319	LEU
1	C	325	LEU
1	C	353	LYS
1	C	358	ARG
1	C	370	PRO

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Mol	Chain	Res	Type
1	C	373	THR
1	D	9	ASP
1	D	21	ILE
1	D	43	VAL
1	D	53	VAL
1	D	56	PRO
1	D	73	LYS
1	D	74	LEU
1	D	77	LEU
1	D	82	THR
1	D	94	MET
1	D	96	LEU
1	D	112	LEU
1	D	117	SER
1	D	125	ILE
1	D	130	THR
1	D	140	THR
1	D	147	LEU
1	D	153	MET
1	D	162	LEU
1	D	171	GLN
1	D	173	ILE
1	D	176	SER
1	D	177	VAL
1	D	210	LYS
1	D	218	ASN
1	D	230	ILE
1	D	233	ARG
1	D	234	LYS
1	D	239	ILE
1	D	240	ILE
1	D	291	VAL
1	D	294	ARG
1	D	303	ASP
1	D	308	LEU
1	D	313	THR
1	D	317	ASP
1	D	318	ILE
1	D	320	PRO
1	D	325	LEU
1	D	358	ARG
1	D	360	LYS

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Mol	Chain	Res	Type
1	D	370	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	80	ASN
1	A	166	ASN
1	A	171	GLN
1	A	218	ASN
1	A	271	HIS
1	A	295	ASN
1	A	352	GLN
1	A	375	GLN
1	B	25	HIS
1	B	80	ASN
1	B	118	HIS
1	B	148	HIS
1	B	166	ASN
1	B	171	GLN
1	B	250	GLN
1	B	352	GLN
1	B	375	GLN
1	C	3	GLN
1	C	67	GLN
1	C	80	ASN
1	C	86	HIS
1	C	101	HIS
1	C	122	ASN
1	C	148	HIS
1	C	166	ASN
1	C	218	ASN
1	C	250	GLN
1	C	295	ASN
1	D	3	GLN
1	D	67	GLN
1	D	80	ASN
1	D	81	HIS
1	D	101	HIS
1	D	122	ASN
1	D	166	ASN
1	D	171	GLN

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Mol	Chain	Res	Type
1	D	218	ASN
1	D	295	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FMN	B	711	-	33,33,33	3.19	14 (42%)	48,50,50	2.38	16 (33%)
3	FEO	A	501	1	0,2,2	-	-	-		
4	FMN	D	731	-	33,33,33	3.04	16 (48%)	48,50,50	2.45	17 (35%)
3	FEO	D	531	1	0,2,2	-	-	-		
4	FMN	A	701	-	33,33,33	3.26	16 (48%)	48,50,50	2.52	16 (33%)
3	FEO	C	521	1	0,2,2	-	-	-		
4	FMN	C	721	-	33,33,33	2.88	13 (39%)	48,50,50	2.46	17 (35%)
3	FEO	B	511	1	0,2,2	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	D	731	-	-	0/18/18/18	0/3/3/3
4	FMN	B	711	-	-	0/18/18/18	0/3/3/3
4	FMN	A	701	-	-	0/18/18/18	0/3/3/3
4	FMN	C	721	-	-	0/18/18/18	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	731	FMN	C9-C9A	7.87	1.52	1.39
4	A	701	FMN	C6-C7	7.65	1.50	1.39
4	B	711	FMN	C9-C9A	7.45	1.51	1.39
4	B	711	FMN	C9A-C5A	7.38	1.53	1.41
4	A	701	FMN	C9A-C5A	7.22	1.52	1.41
4	B	711	FMN	C6-C7	7.08	1.49	1.39
4	C	721	FMN	C9-C9A	7.05	1.51	1.39
4	D	731	FMN	C9A-C5A	6.88	1.52	1.41
4	A	701	FMN	C9-C9A	6.82	1.50	1.39
4	D	731	FMN	C6-C7	6.41	1.48	1.39
4	C	721	FMN	C6-C7	5.97	1.47	1.39
4	B	711	FMN	C2-N3	5.95	1.52	1.39
4	C	721	FMN	C9A-C5A	5.94	1.50	1.41
4	A	701	FMN	C2-N3	5.70	1.51	1.39
4	D	731	FMN	C4A-C10	4.93	1.58	1.44
4	D	731	FMN	C2-N3	4.93	1.49	1.39
4	A	701	FMN	C4A-C10	4.90	1.58	1.44
4	B	711	FMN	C4-N3	4.87	1.48	1.38
4	C	721	FMN	C2-N3	4.79	1.49	1.39
4	A	701	FMN	C6-C5A	4.71	1.47	1.40
4	B	711	FMN	C4A-C10	4.60	1.57	1.44
4	C	721	FMN	C4A-C10	4.33	1.56	1.44
4	C	721	FMN	C4-N3	4.29	1.46	1.38
4	D	731	FMN	C4-N3	4.24	1.46	1.38
4	B	711	FMN	C6-C5A	4.19	1.46	1.40
4	A	701	FMN	C5A-N5	4.08	1.46	1.39
4	A	701	FMN	C4-N3	3.96	1.46	1.38
4	C	721	FMN	C6-C5A	3.76	1.45	1.40
4	C	721	FMN	C2'-C3'	-3.70	1.47	1.53
4	D	731	FMN	C6-C5A	3.56	1.45	1.40
4	A	701	FMN	C2'-C3'	-3.48	1.47	1.53
4	C	721	FMN	C5A-N5	3.33	1.45	1.39
4	B	711	FMN	C5A-N5	3.28	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	FMN	C8-C7	3.24	1.48	1.40
4	D	731	FMN	C5A-N5	3.22	1.45	1.39
4	A	701	FMN	C5'-C4'	3.20	1.56	1.51
4	C	721	FMN	C5'-C4'	3.19	1.56	1.51
4	D	731	FMN	C5'-C4'	3.11	1.56	1.51
4	B	711	FMN	C8-C7	3.05	1.48	1.40
4	A	701	FMN	O3'-C3'	2.94	1.50	1.43
4	D	731	FMN	O3'-C3'	2.79	1.49	1.43
4	C	721	FMN	C8-C7	2.72	1.47	1.40
4	D	731	FMN	C10-N1	2.71	1.38	1.33
4	A	701	FMN	C4A-N5	2.68	1.36	1.30
4	A	701	FMN	C10-N1	2.67	1.38	1.33
4	D	731	FMN	C8M-C8	-2.65	1.46	1.51
4	B	711	FMN	C5'-C4'	2.62	1.55	1.51
4	C	721	FMN	P-O2P	-2.46	1.45	1.54
4	D	731	FMN	C8-C7	2.35	1.46	1.40
4	B	711	FMN	C8M-C8	-2.35	1.46	1.51
4	B	711	FMN	C1'-C2'	2.35	1.55	1.52
4	A	701	FMN	P-O1P	2.32	1.57	1.50
4	B	711	FMN	C2'-C3'	-2.29	1.49	1.53
4	D	731	FMN	P-O5'	-2.23	1.53	1.60
4	B	711	FMN	P-O2P	-2.15	1.46	1.54
4	D	731	FMN	C10-N10	2.15	1.42	1.37
4	C	721	FMN	O3'-C3'	2.10	1.48	1.43
4	D	731	FMN	P-O2P	-2.09	1.47	1.54
4	A	701	FMN	C10-N10	2.08	1.41	1.37

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	FMN	C5A-C9A-N10	8.14	125.33	117.97
4	D	731	FMN	C5A-C9A-N10	7.26	124.54	117.97
4	C	721	FMN	C5A-C9A-N10	7.04	124.33	117.97
4	B	711	FMN	C5A-C9A-N10	6.98	124.28	117.97
4	A	701	FMN	C9A-C5A-N5	-6.11	115.97	122.45
4	C	721	FMN	C7M-C7-C6	-6.00	109.00	119.57
4	D	731	FMN	C7M-C7-C6	-5.84	109.28	119.57
4	C	721	FMN	C9A-C5A-N5	-5.62	116.49	122.45
4	B	711	FMN	C7M-C7-C6	-5.56	109.78	119.57
4	B	711	FMN	C9A-C5A-N5	-5.49	116.63	122.45
4	D	731	FMN	C9A-C5A-N5	-5.27	116.86	122.45
4	C	721	FMN	C7M-C7-C8	5.22	131.41	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	FMN	C7M-C7-C6	-5.18	110.44	119.57
4	B	711	FMN	C7M-C7-C8	4.71	130.38	120.76
4	D	731	FMN	C7M-C7-C8	4.70	130.36	120.76
4	A	701	FMN	C7M-C7-C8	4.41	129.77	120.76
4	A	701	FMN	O2-C2-N1	4.36	129.04	121.80
4	D	731	FMN	O2-C2-N1	4.33	128.98	121.80
4	C	721	FMN	O2-C2-N1	4.26	128.87	121.80
4	C	721	FMN	C10-N1-C2	4.15	125.84	116.85
4	B	711	FMN	C10-N1-C2	4.07	125.66	116.85
4	B	711	FMN	O2-C2-N1	4.03	128.49	121.80
4	A	701	FMN	C10-N1-C2	3.86	125.21	116.85
4	A	701	FMN	C6-C5A-N5	3.82	124.79	118.44
4	D	731	FMN	C10-N1-C2	3.77	125.02	116.85
4	C	721	FMN	O4-C4-N3	-3.59	113.37	120.11
4	A	701	FMN	O4-C4-N3	-3.56	113.42	120.11
4	D	731	FMN	O4-C4-N3	-3.31	113.88	120.11
4	D	731	FMN	C9A-N10-C10	-3.26	115.79	120.75
4	D	731	FMN	C6-C5A-N5	3.22	123.78	118.44
4	A	701	FMN	C9-C9A-N10	-3.13	117.64	121.85
4	C	721	FMN	C6-C5A-N5	3.13	123.64	118.44
4	C	721	FMN	C9A-N10-C10	-3.11	116.01	120.75
4	C	721	FMN	C1'-N10-C9A	3.06	126.57	120.63
4	B	711	FMN	C9A-N10-C10	-3.03	116.13	120.75
4	C	721	FMN	C4A-C10-N10	2.96	120.72	116.48
4	D	731	FMN	C4A-C10-N1	-2.95	117.37	124.59
4	B	711	FMN	C6-C5A-N5	2.87	123.22	118.44
4	A	701	FMN	C9A-N10-C10	-2.87	116.38	120.75
4	D	731	FMN	O2-C2-N3	-2.85	113.12	118.58
4	C	721	FMN	C4A-C10-N1	-2.79	117.75	124.59
4	B	711	FMN	C4A-C10-N10	2.73	120.39	116.48
4	B	711	FMN	C1'-N10-C9A	2.71	125.91	120.63
4	D	731	FMN	C4A-C10-N10	2.69	120.33	116.48
4	B	711	FMN	C4'-C3'-C2'	2.65	117.98	113.57
4	B	711	FMN	C4A-C10-N1	-2.64	118.12	124.59
4	A	701	FMN	C4A-C10-N10	2.59	120.19	116.48
4	A	701	FMN	C4A-C10-N1	-2.59	118.24	124.59
4	D	731	FMN	O3'-C3'-C4'	-2.53	103.19	108.93
4	C	721	FMN	O2-C2-N3	-2.53	113.74	118.58
4	A	701	FMN	C1'-N10-C9A	2.51	125.50	120.63
4	A	701	FMN	C4'-C3'-C2'	2.49	117.72	113.57
4	D	731	FMN	C1'-N10-C9A	2.47	125.43	120.63
4	C	721	FMN	C5A-N5-C4A	2.36	121.91	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	711	FMN	O3'-C3'-C4'	-2.35	103.60	108.93
4	C	721	FMN	C9A-C9-C8	2.29	123.83	119.22
4	C	721	FMN	C9-C9A-C5A	-2.26	116.03	120.03
4	A	701	FMN	C9A-C9-C8	2.22	123.69	119.22
4	B	711	FMN	O4-C4-N3	-2.21	115.97	120.11
4	A	701	FMN	O2-C2-N3	-2.14	114.47	118.58
4	B	711	FMN	C4-C4A-C10	2.13	120.58	116.93
4	D	731	FMN	C9-C9A-N10	-2.10	119.03	121.85
4	C	721	FMN	C10-C4A-N5	-2.09	120.53	124.81
4	D	731	FMN	C5A-N5-C4A	2.06	121.43	118.09
4	D	731	FMN	C9-C9A-C5A	-2.04	116.43	120.03
4	B	711	FMN	C9-C9A-N10	-2.03	119.12	121.85

There are no chirality outliers.

There are no torsion outliers.

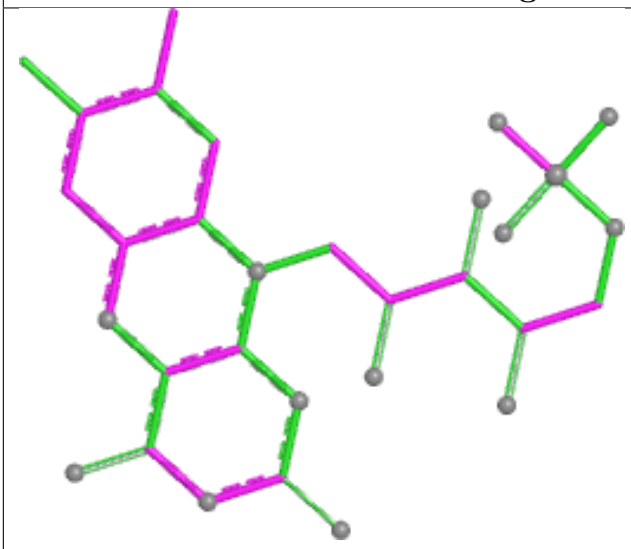
There are no ring outliers.

2 monomers are involved in 4 short contacts:

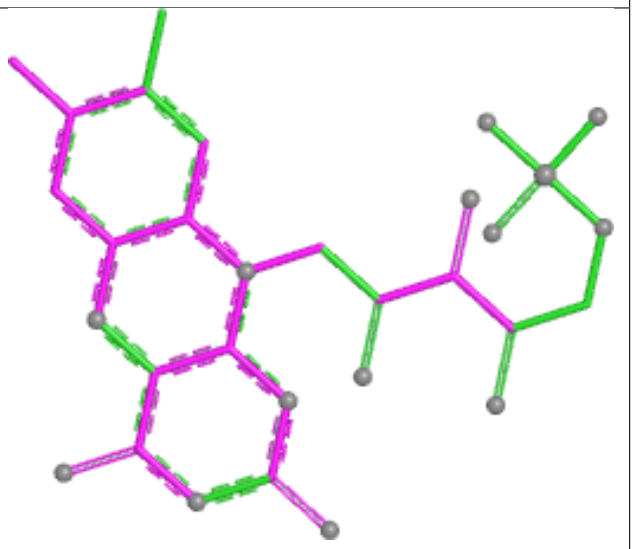
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	711	FMN	2	0
4	C	721	FMN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

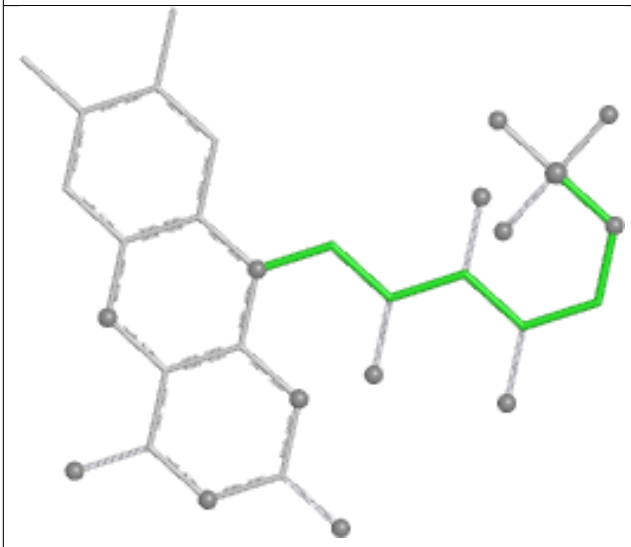
Ligand FMN B 711



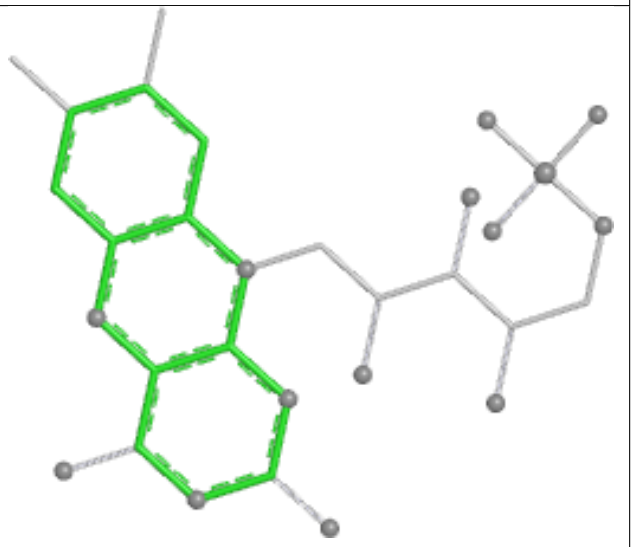
Bond lengths



Bond angles

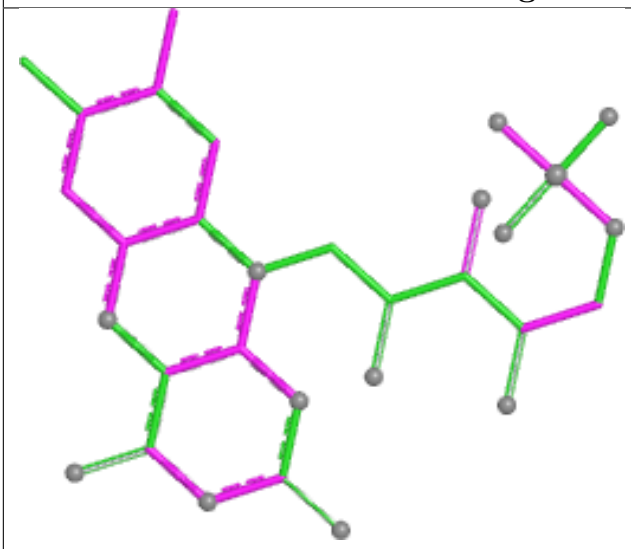


Torsions

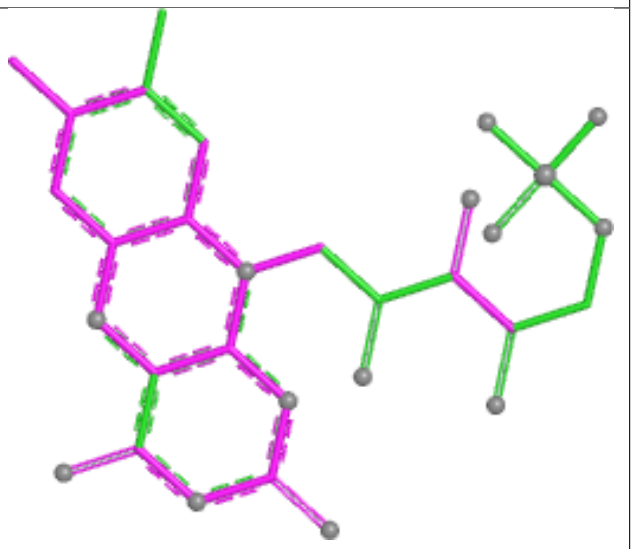


Rings

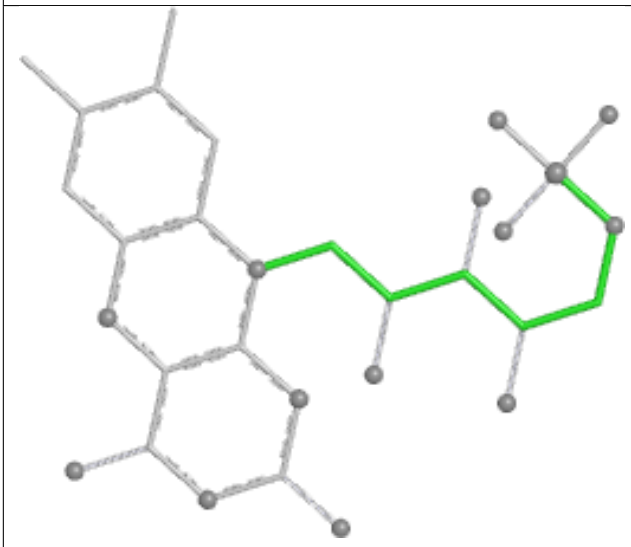
Ligand FMN D 731



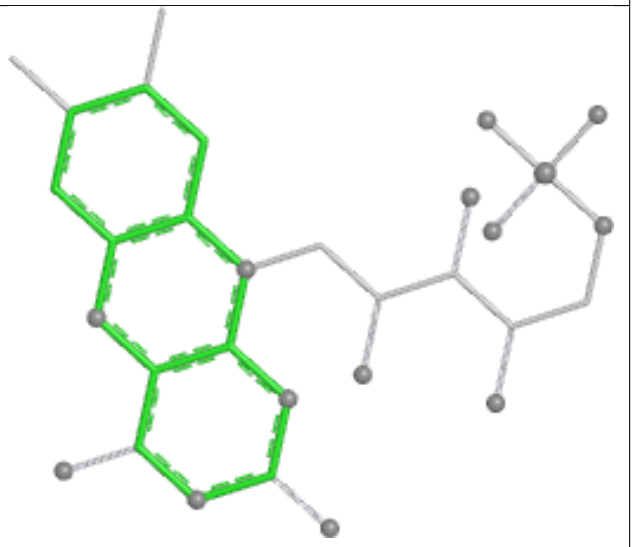
Bond lengths



Bond angles

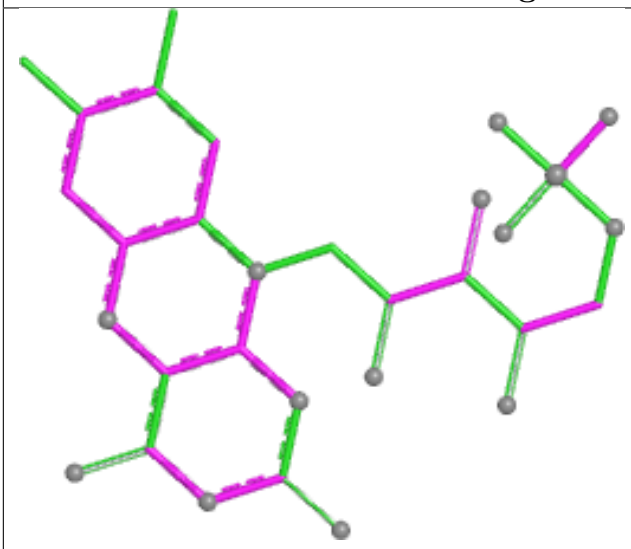


Torsions

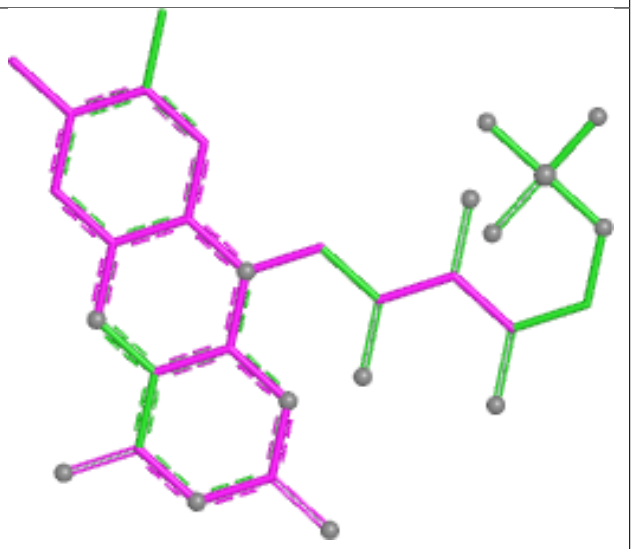


Rings

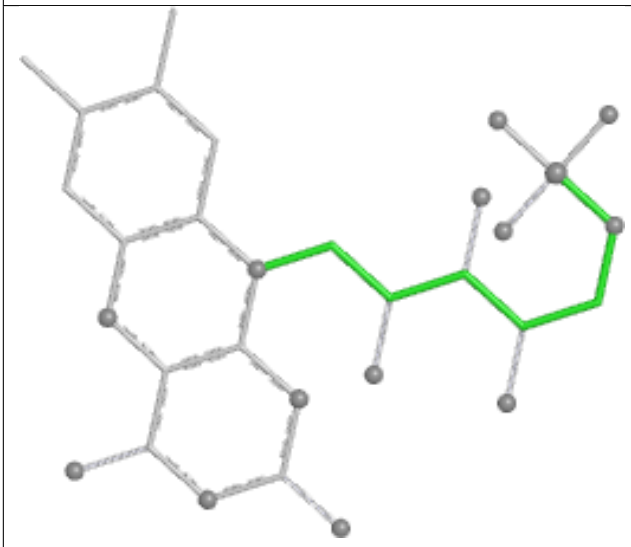
Ligand FMN A 701



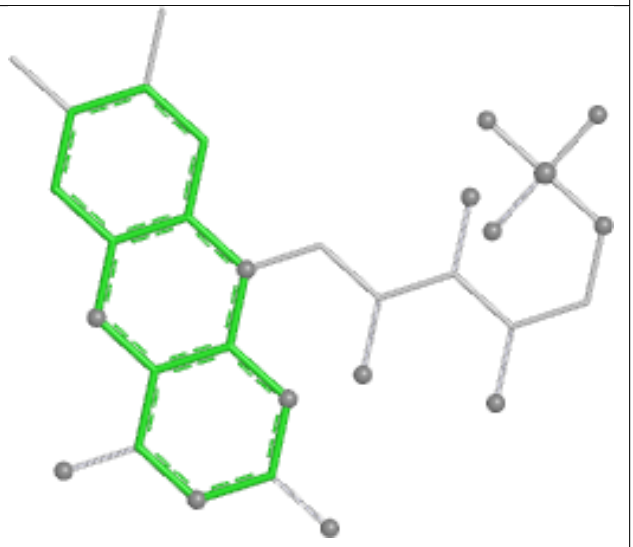
Bond lengths



Bond angles

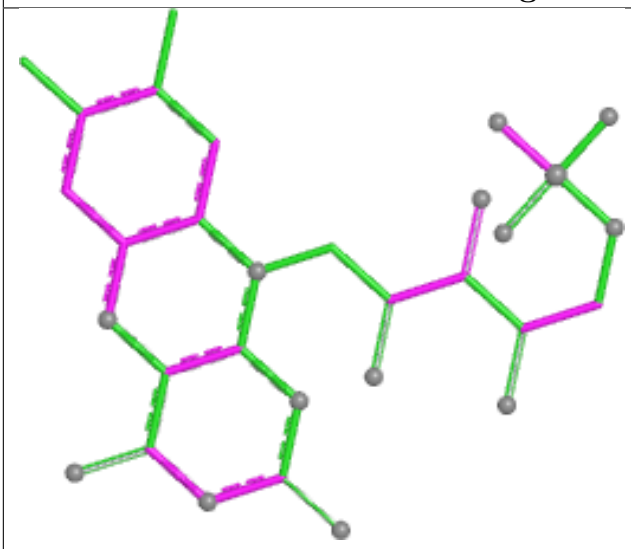


Torsions

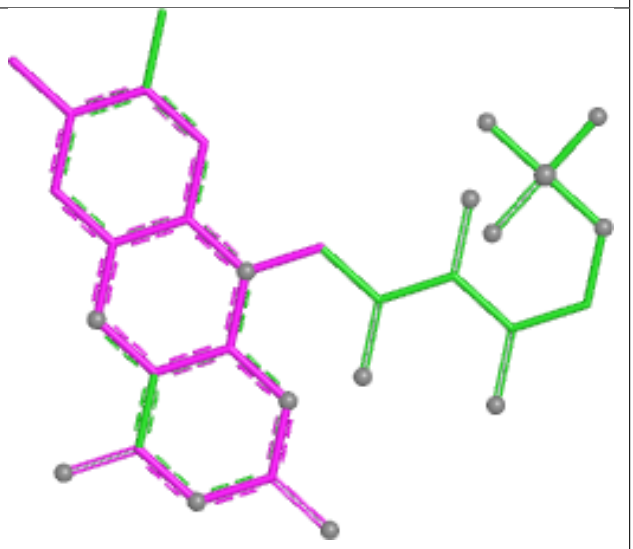


Rings

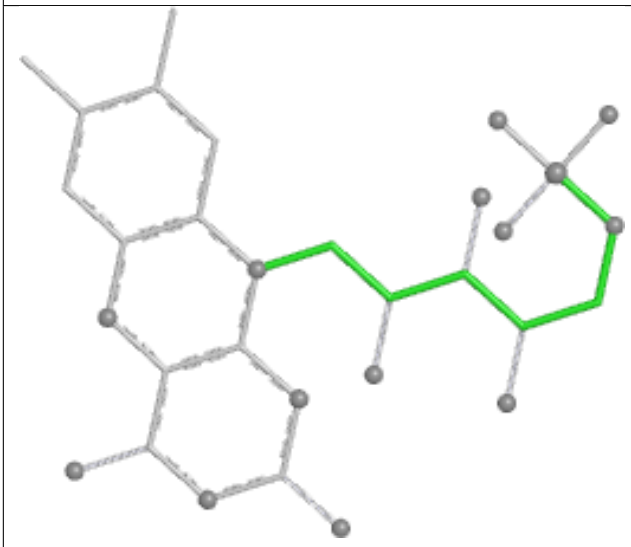
Ligand FMN C 721



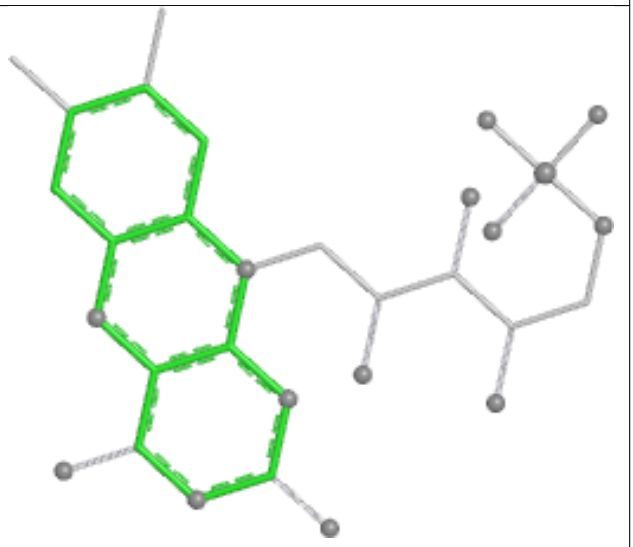
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	398/398 (100%)	0.27	16 (4%)	42	33	45, 67, 85, 99	0
1	B	398/398 (100%)	0.43	19 (4%)	35	28	48, 69, 93, 104	0
1	C	398/398 (100%)	0.06	10 (2%)	58	48	43, 57, 77, 91	0
1	D	398/398 (100%)	0.05	14 (3%)	47	38	43, 57, 77, 92	0
All	All	1592/1592 (100%)	0.20	59 (3%)	45	36	43, 62, 85, 104	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	ASP	5.1
1	D	118	HIS	4.8
1	D	73	LYS	3.5
1	B	121	PHE	3.2
1	C	245	ARG	3.1
1	A	118	HIS	3.0
1	D	71	PRO	2.9
1	C	117	SER	2.9
1	D	3	GLN	2.8
1	A	217	ILE	2.8
1	A	28	ALA	2.8
1	B	123	TYR	2.8
1	B	357	GLU	2.7
1	C	26	GLY	2.6
1	D	120	ASP	2.6
1	D	32	HIS	2.5
1	B	217	ILE	2.5
1	A	45	ASP	2.5
1	D	282	CYS	2.5
1	D	234	LYS	2.5
1	B	96	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	74	LEU	2.4
1	D	117	SER	2.4
1	B	95	GLU	2.4
1	B	43	VAL	2.4
1	B	216	LYS	2.4
1	C	381	GLU	2.4
1	C	380	GLY	2.4
1	D	370	PRO	2.4
1	A	122	ASN	2.3
1	C	234	LYS	2.3
1	B	69	LYS	2.3
1	C	379	ARG	2.3
1	B	346	GLY	2.3
1	B	73	LYS	2.3
1	A	124	THR	2.3
1	D	216	LYS	2.3
1	A	216	LYS	2.2
1	A	252	LYS	2.2
1	D	399	ASP	2.2
1	A	282	CYS	2.2
1	D	45	ASP	2.2
1	C	370	PRO	2.2
1	B	10	GLY	2.2
1	A	238	ARG	2.2
1	A	397	ILE	2.2
1	B	47	THR	2.2
1	C	118	HIS	2.2
1	A	357	GLU	2.1
1	A	234	LYS	2.1
1	A	117	SER	2.1
1	A	139	LEU	2.1
1	B	124	THR	2.1
1	B	373	THR	2.1
1	D	379	ARG	2.1
1	B	102	VAL	2.1
1	B	98	PRO	2.1
1	A	138	SER	2.0
1	C	398	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

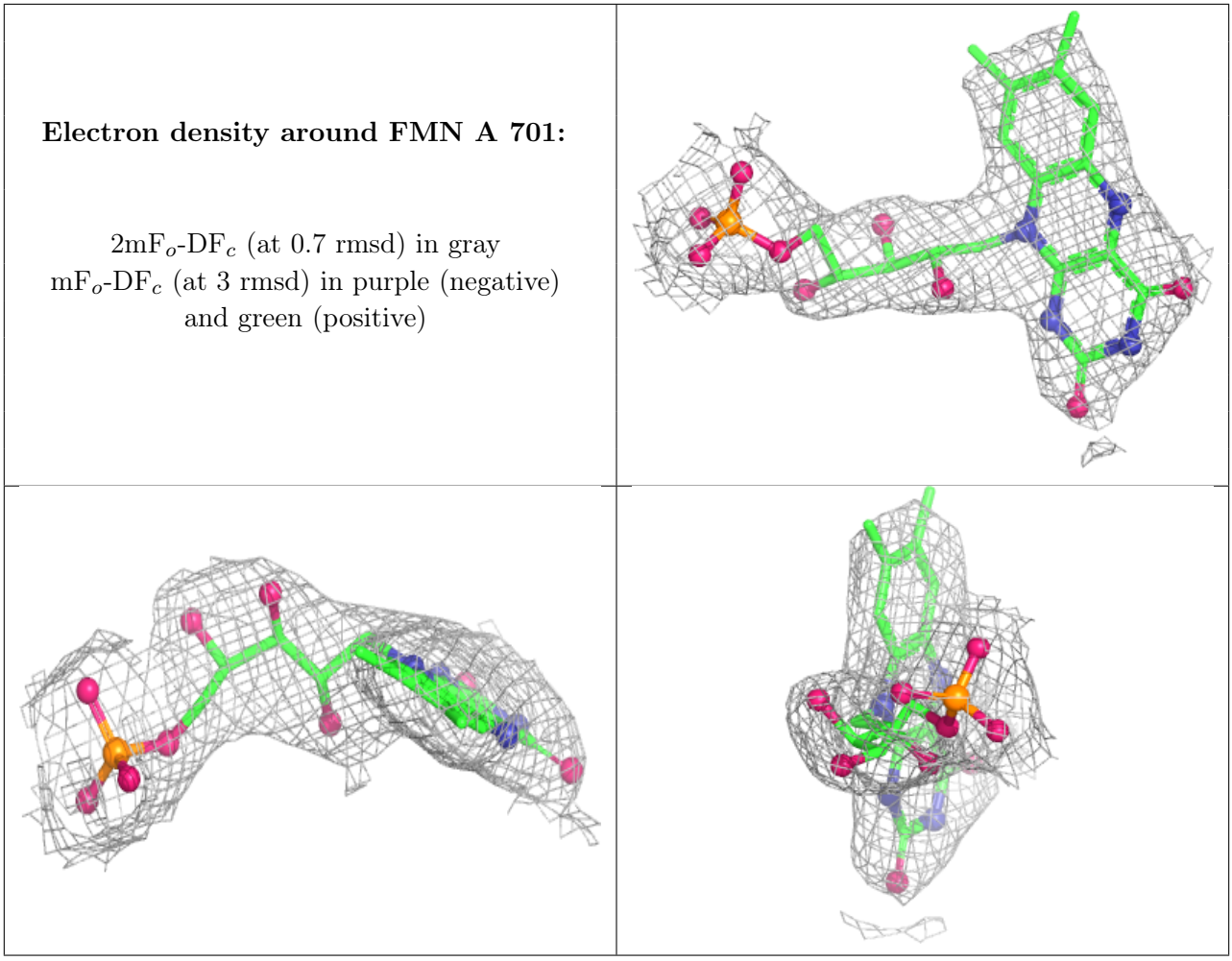
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMN	A	701	31/31	0.96	0.09	63,70,73,75	0
4	FMN	D	731	31/31	0.96	0.08	51,53,59,59	0
4	FMN	C	721	31/31	0.97	0.08	50,53,57,60	0
4	FMN	B	711	31/31	0.97	0.09	59,72,76,76	0
2	ZN	B	610	1/1	0.98	0.05	90,90,90,90	0
2	ZN	C	621	1/1	0.99	0.05	96,96,96,96	0
2	ZN	D	631	1/1	0.99	0.03	92,92,92,92	0
3	FEO	A	501	3/3	0.99	0.04	59,59,61,63	0
3	FEO	B	511	3/3	0.99	0.05	59,59,62,65	0
3	FEO	C	521	3/3	0.99	0.03	45,45,46,48	0
2	ZN	A	601	1/1	0.99	0.04	82,82,82,82	0
2	ZN	A	600	1/1	0.99	0.03	91,91,91,91	0
2	ZN	B	611	1/1	0.99	0.04	86,86,86,86	0
2	ZN	C	620	1/1	0.99	0.04	80,80,80,80	0
2	ZN	D	630	1/1	1.00	0.02	81,81,81,81	0
3	FEO	D	531	3/3	1.00	0.03	48,48,48,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

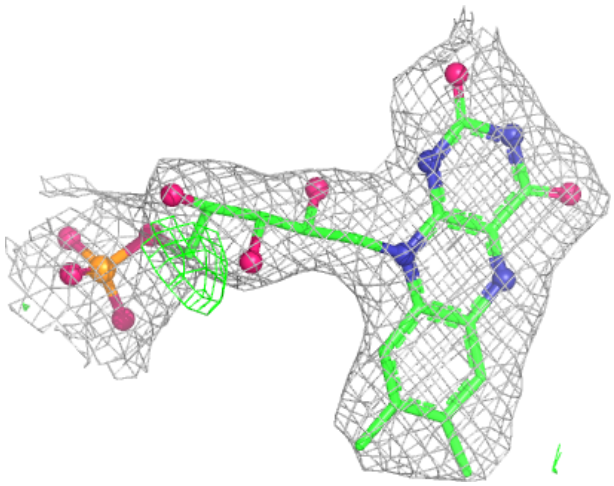
Electron density around FMN A 701:

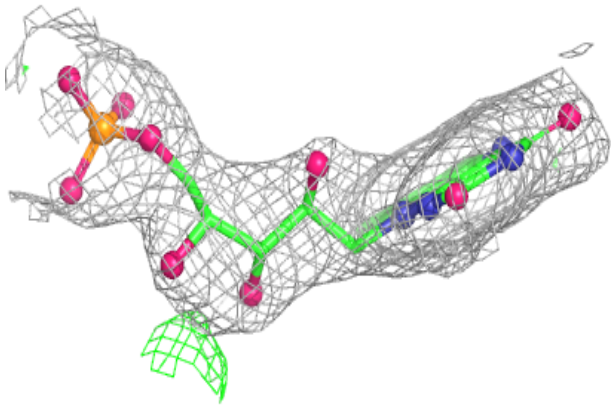
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

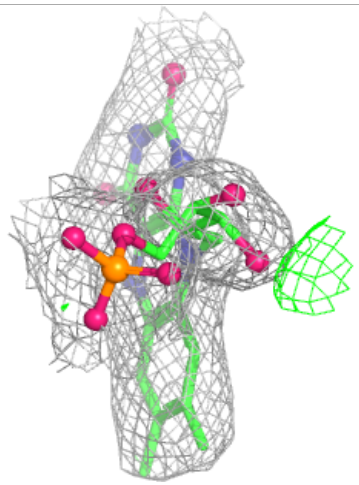


Electron density around FMN D 731:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

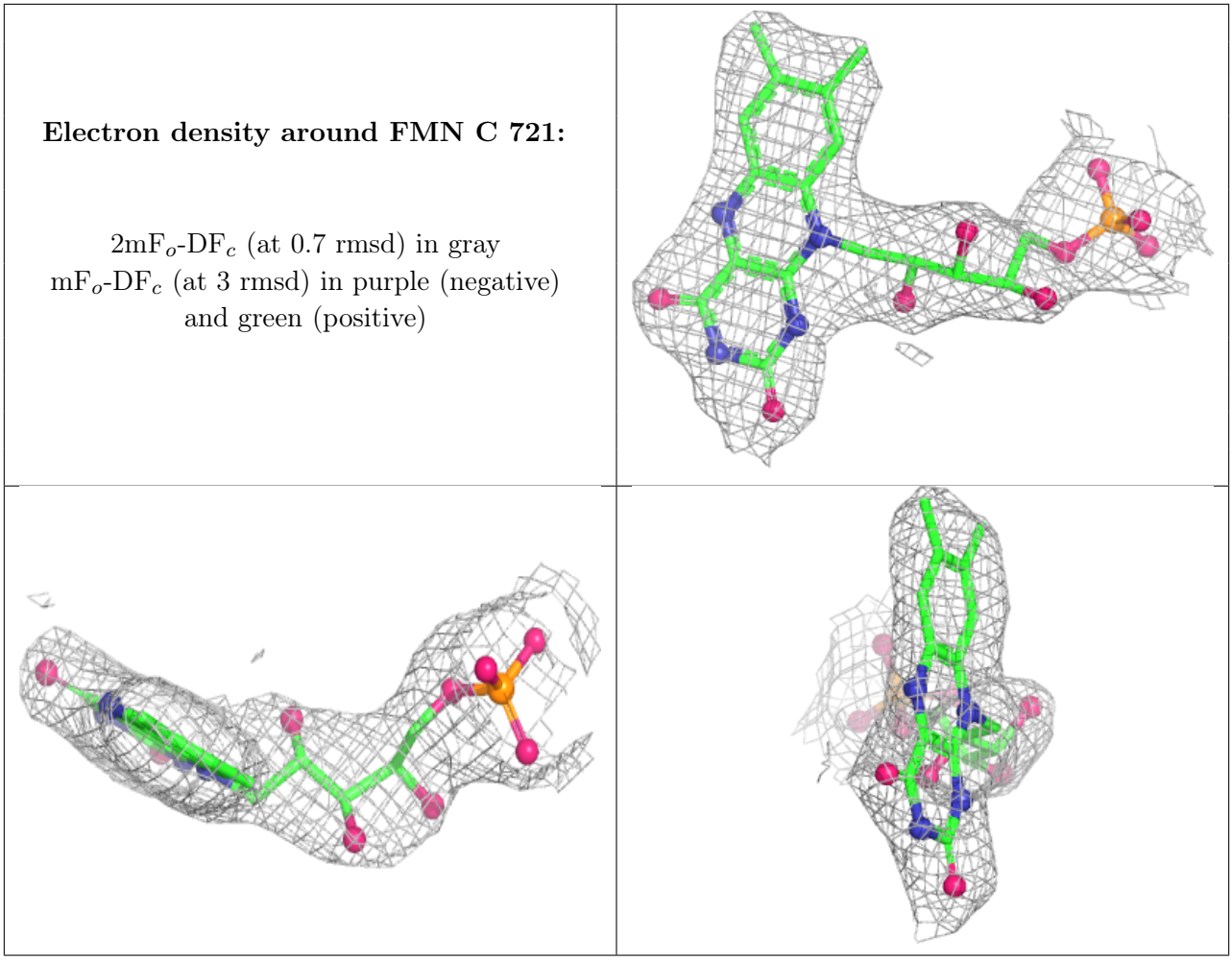






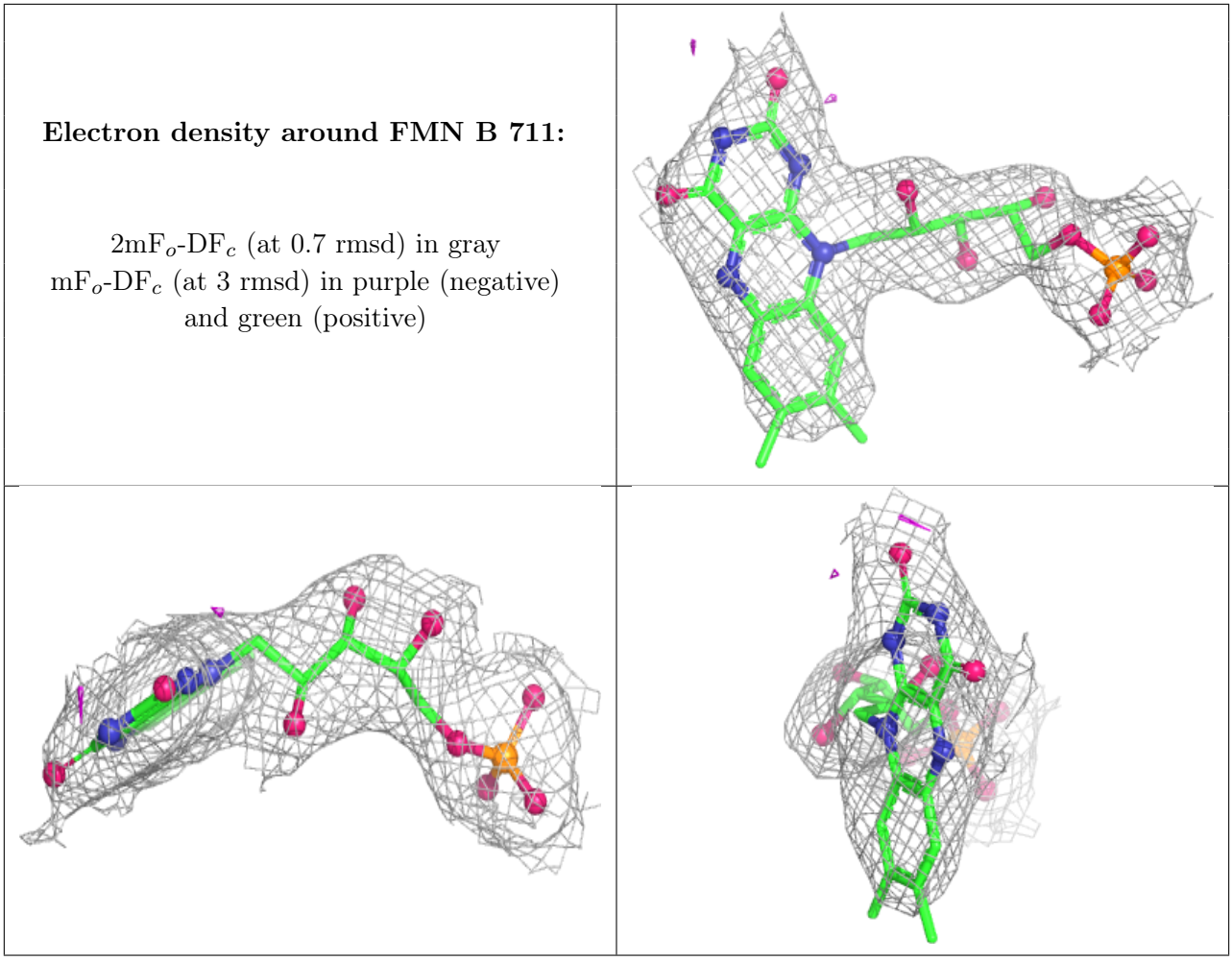
Electron density around FMN C 721:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FMN B 711:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.